```
=> fil casreact
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FILE CONTENT:1840 - 19 Jun 2005 VOL 142 ISS 25

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*                                                        *
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*                                                        *
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provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d que l13
L1              STR

RRT 8                RRT 4                PRO 12
    G2                   X                    H
     \                   |                    |
      \                  |2                   |
G2~S~O           G1~C~X           G1~C#O
5  6  7          1  |  3           9  10 11
                     H
                    13

VAR G1=AK/CY
VAR G2=AK/CY
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   6
CONNECT IS E1  RC AT   7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE

  ****MAPPINGS****
NOD SYM      ROL    NOD SYM      ROL
  2 C        RRT     10 C        PRO
 10 C        PRO      2 C        RRT
L11        2583 SEA FILE=CASREACT ABB=ON  PLU=ON  ALDEHYDE/FG.PRO (L) (SULFOXID
```

E/FG.RCT OR SULFOXIDE/FG.RGT)
L13 12 SEA FILE=CASREACT SUB=L11 SSS FUL L1 (130 REACTIONS)

=> d l13 ibib abs crd 1-12

L13 ANSWER 1 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:164928 CASREACT
TITLE: Synthesis and biological evaluation of novel leucomycin analogues modified at the C-3 position. I. Epimerization and methylation of the 3-hydroxyl group
AUTHOR(S): Furuuchi, Takeshi; Kurihara, Ken-Ichi; Yoshida, Takuji; Ajito, Keiichi
CORPORATE SOURCE: Pharmaceutical Research Center, Meiji Seika Kaisha, Ltd., Yokohama, 222-8567, Japan
SOURCE: Journal of Antibiotics (2003), 56(4), 399-414
CODEN: JANTAJ; ISSN: 0021-8820
PUBLISHER: Japan Antibiotics Research Association
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis and biol. evaluation of sixteen-membered macrolides modified at the C-3 position are described. 3-Epi-leucomycin A7, 3-O-acyl-3-epi-leucomycin A7 analogs, 3-O-acylleucomycin A7 analogs and 3-O-methylleucomycin analogs were synthesized via fully protected intermediates. After appropriate modification, subsequent deprotections were performed to furnish a variety of leucomycin analogs. Methylation of the 3-hydroxyl group was found to improve the pharmacoprofile of leucomycin antibiotics. 3-O-Methylrokitamycin (I) showed enhanced antibacterial activity in vitro and 3,3''-di-O-methyl-4''-O-(3-methylbutyl)leucomycin V (II) exhibited improved metabolic stability in rat plasma in vitro.

RX(111) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(112) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(113) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(114) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(115) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(116) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(123) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(130) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(137) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(139) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(140) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(141) OF 182 - REACTION DIAGRAM NOT AVAILABLE

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RX(143) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(144) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(145) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(146) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(147) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(148) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(149) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(150) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(151) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(152) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(153) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(154) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(155) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(156) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(162) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(164) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(165) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(166) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(167) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(168) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(169) OF 182 - REACTION DIAGRAM NOT AVAILABLE

RX(175) OF 182 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:338079 CASREACT
TITLE: Conformationally constrained analogues of diacylglycerol (DAG). Part 19: Asymmetric syntheses of (3R)- and (3S)-3-hydroxy-4,4-disubstituted

heptono-1,4-lactones as protein kinase C (PK-C) ligands with increased hydrophilicity

AUTHOR(S): Nacro, Kassoum; Lee, Jeewoo; Barchi, Joseph J.; Lewin, Nancy E.; Blumberg, Peter M.; Marquez, Victor E.

CORPORATE SOURCE: Center for Cancer Research, Laboratory of Medicinal Chemistry, National Cancer Institute at Frederick, Frederick, MD, 21702, USA

SOURCE: Tetrahedron (2002), 58(26), 5335-5345
CODEN: TETRAB; ISSN: 0040-4020

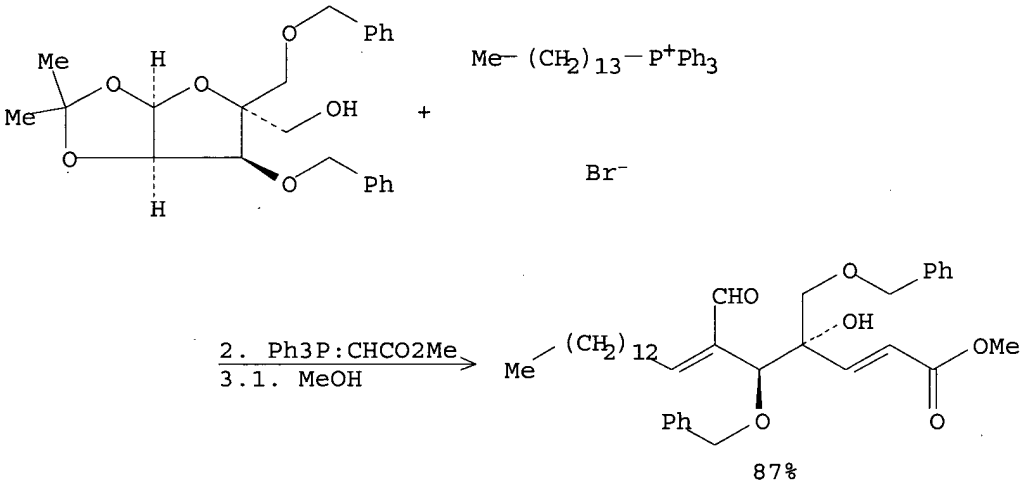
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

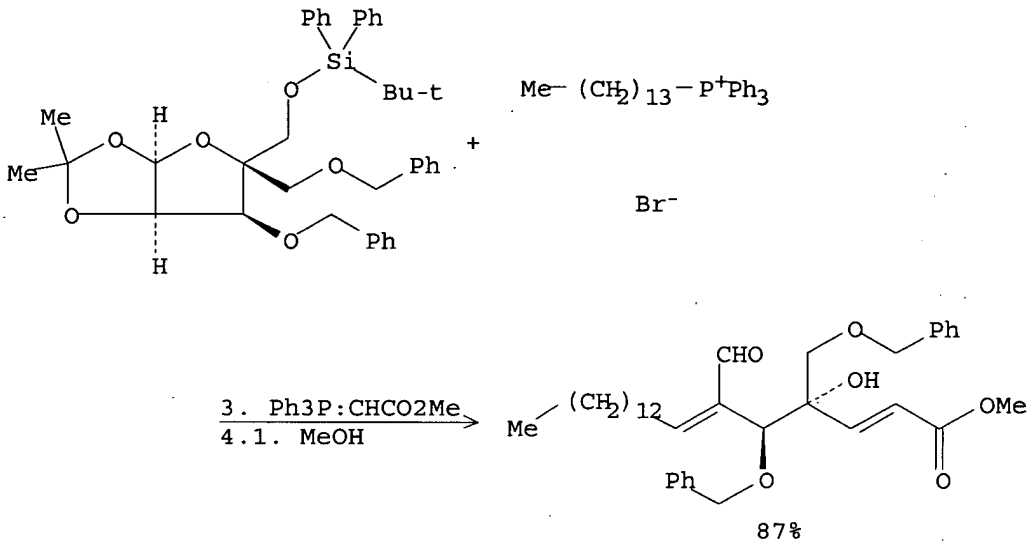
AB The stereospecific introduction of (R)- and (S)-OH groups at position C-3 of two diacylglycerol γ-lactones (DAG-lactones) previously identified as strong protein kinase C (PK-C) ligands is presented. The compds. were designed to investigate whether the extra OH group in a specific orientation could establish an addnl. hydrogen bond with the C1 domain of PK-C, thus providing a DAG analog with reduced lipophilicity. The OH groups were introduced following two different diastereoselective multistep syntheses starting from diacetone-d-glucose. The PK-C binding affinities for the new compds. were weaker in comparison to those of the parent compds., suggesting that the extra OH does not engage efficiently in hydrogen bonding at the receptor.

RX(163) OF 213 - 6 STEPS



NOTE: 3) other product also detected, second anomer was not characterized, yield of second anomer was 23%, 4) Swern oxidation

RX(164) OF 213 - 7 STEPS



87%

NOTE: 4) other product also detected, second anomer was not characterized, yield of second anomer was 23%, 5) Swern oxidation

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 12 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 132:137730 CASREACT

TITLE: Preparation of derivatized resins useful for solid-phase peptide synthesis, combinatorial chemistry, and peptide or protein purification and separation

INVENTOR(S): Siev, Daniel V.; Semple, J. Edward; Weinhouse, Michael I.

PATENT ASSIGNEE(S): Corvas International Inc., USA

SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000005243	A2	20000203	WO 1999-US16828	19990723
WO 2000005243	A3	20000420		

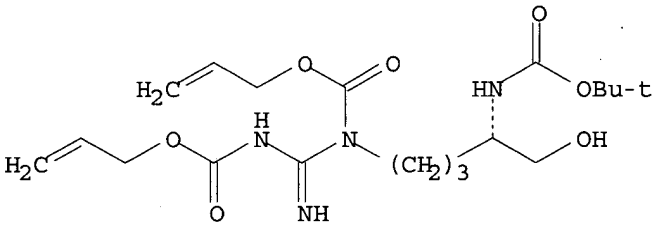
W: JP
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE

US 6787612	B1	20040907	US 1998-122576	19980724
EP 1100812	A2	20010523	EP 1999-935908	19990723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002521385	T2	20020716	JP 2000-561199	19990723
PRIORITY APPLN. INFO.:			US 1998-122576	19980724
			WO 1999-US16828	19990723

AB This invention provides a method for producing a derivatized resin of formula R4NH(C:X)Y-Z-SS [R4 = (un)protected NH2 or OH; X = O, S, NR7; R7 = H, alkyl, alkenyl, aryl, aralkyl, cycloalkyl, heterocyclyl; Y = absent, NH, CH2; Z = absent, NH, O, CO, S, SO2, alkyl, alkenyl, aryl, aralkyl, cycloalkyl, heterocyclyl, and combinations thereof, with provisos; SS = solid support], useful in the arts of solid-phase peptide synthesis, combinatorial chemical, and peptide or protein purification and separation Methods for synthesizing the derivatized resin, the prototypical example of which is hydrazyl-carbonyl-aminomethylated polystyrene (HCAM resin), are disclosed. Thus, aminomethylated polystyrene was coupled with t-Bu carbazate using 1,1-carbonyldiimidazole in DMF and deprotected with DCM/TFA to give HCAM resin. Alternatively, HCAM resin was also prepared by coupling of hydrazine to aminomethylated polystyrene using 1,1-carbonyldiimidazole in DMF. Reaction of an aldehyde or ketoamide with the free amino group of the resin results in an immobilized product, through a semicarbazone moiety, which can be manipulated using standard solid-phase peptide synthetic methods. As opposed to known methods for peptide aldehyde or ketoamide synthesis, the process of this invention provides, among other benefits, a method of solid-phase peptide or peptide analog synthesis that minimizes the amount of solution phase synthetic steps required.

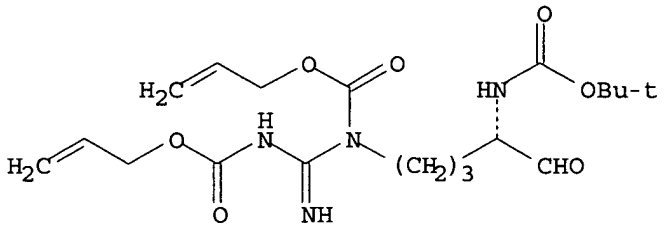
RX(22) OF 249



(step 1)

1. Cl2CHCO2H, EDAP, DMSO, CH2Cl2
2. Water
3. Et2O

RX(22) OF 249



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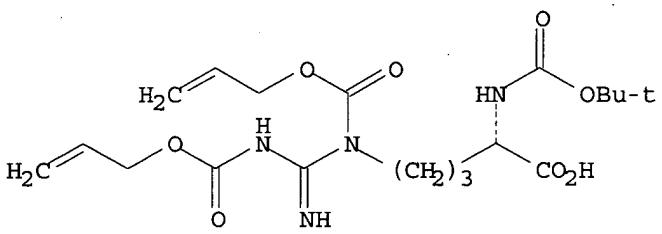
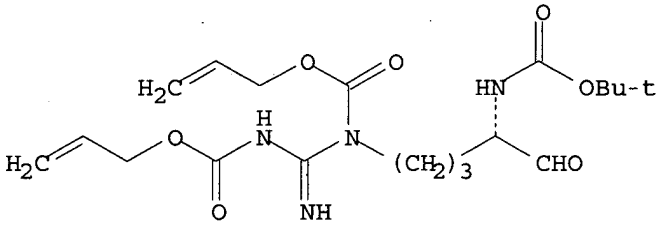
NOTE: STEREOSELECTIVE

RX(38) OF 249 - 2 STEPS



1.1. Et3N, ClCO2Bu-i, THF
1.2. Pyridine
1.3. Water
1.4. HCl
1.5. AcOEt
2.1. Cl2CHCO2H, EDAP, DMSO, CH2Cl2
2.2. Water
2.3. Et2O

RX(38) OF 249 - 2 STEPS



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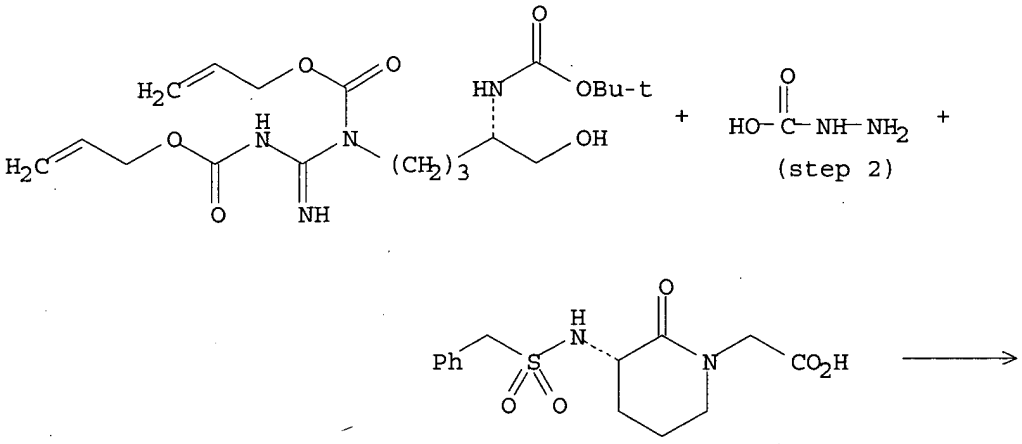
NOTE: 1) STEREOSELECTIVE, 2) STEREOSELECTIVE

RX(163) OF 249 - 6 STEPS



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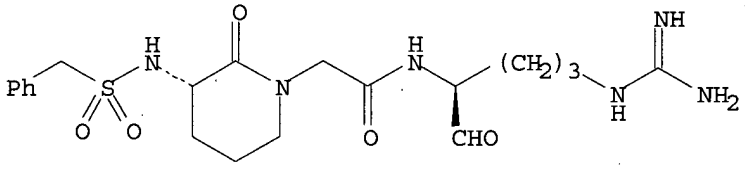

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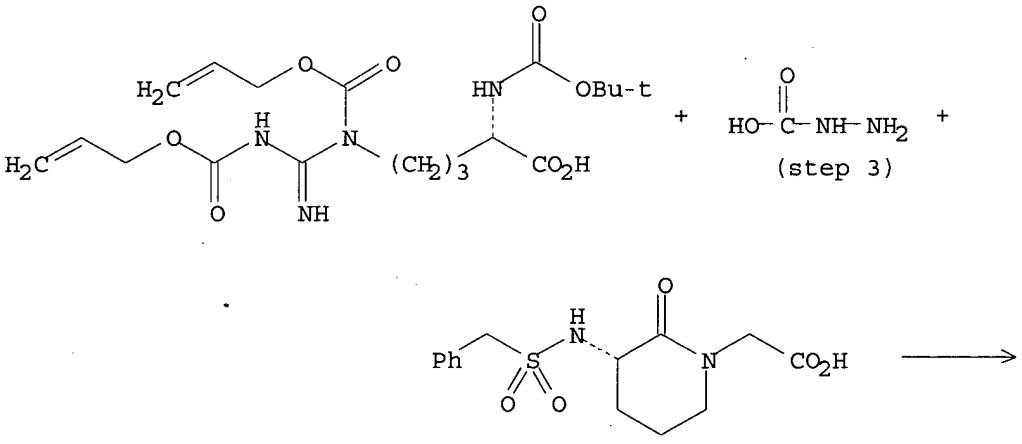
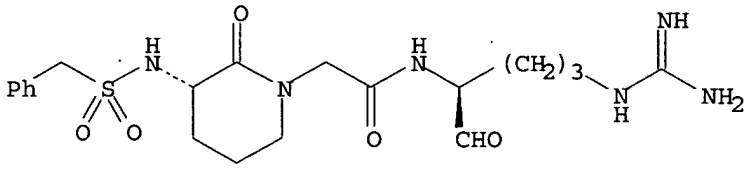
NOTE: 1) STEREOSELECTIVE, 2) RESIN SUPPORTED REACTION, 3) RESIN SUPPORTED REACTION, 4) RESIN SUPPORTED REACTION, 5) RESIN SUPPORTED REACTION, 6) RESIN SUPPORTED REACTION

RX(164) OF 249 - 7 STEPS



RX(164) OF 249 - 7 STEPS



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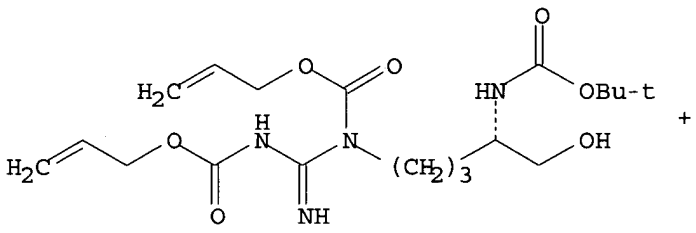
NOTE: 1) STEREOSELECTIVE, 2) STEREOSELECTIVE, 3) RESIN SUPPORTED REACTION, 4) RESIN SUPPORTED REACTION, 5) RESIN SUPPORTED REACTION, 6) RESIN SUPPORTED REACTION, 7) RESIN SUPPORTED REACTION

RX(206) OF 249 - 7 STEPS



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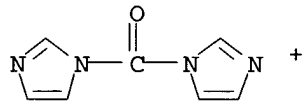

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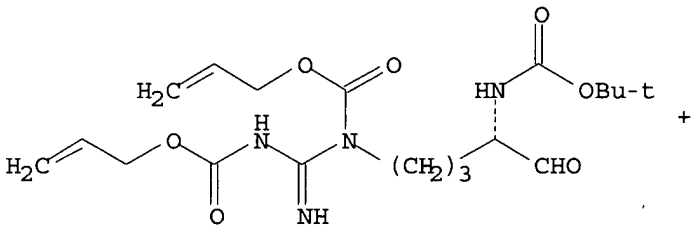

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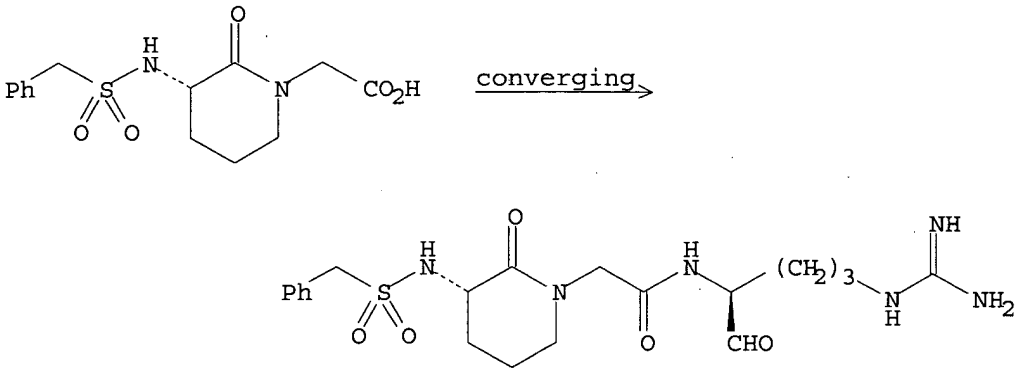

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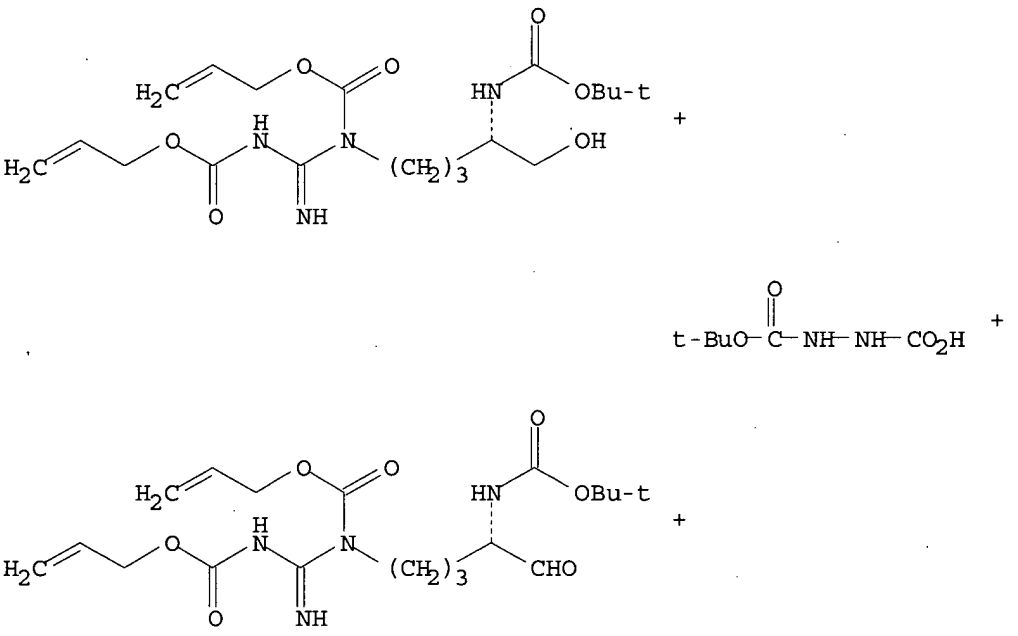
NOTE: RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, STEREOSELECTIVE

RX(208) OF 249 - 7 STEPS



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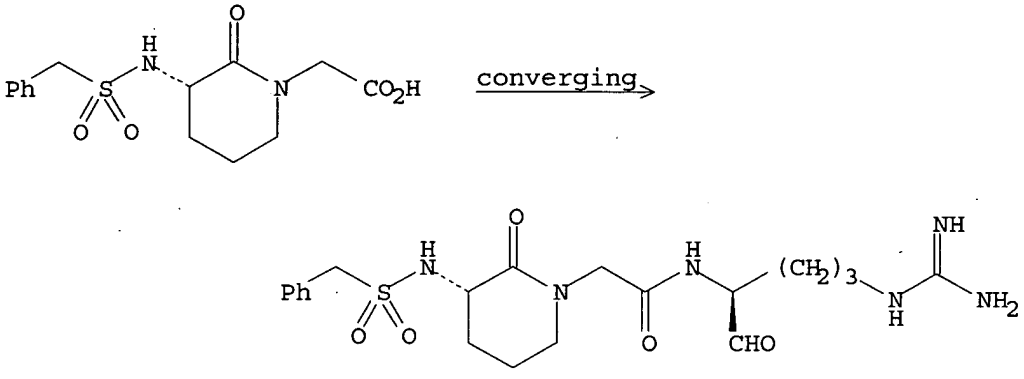

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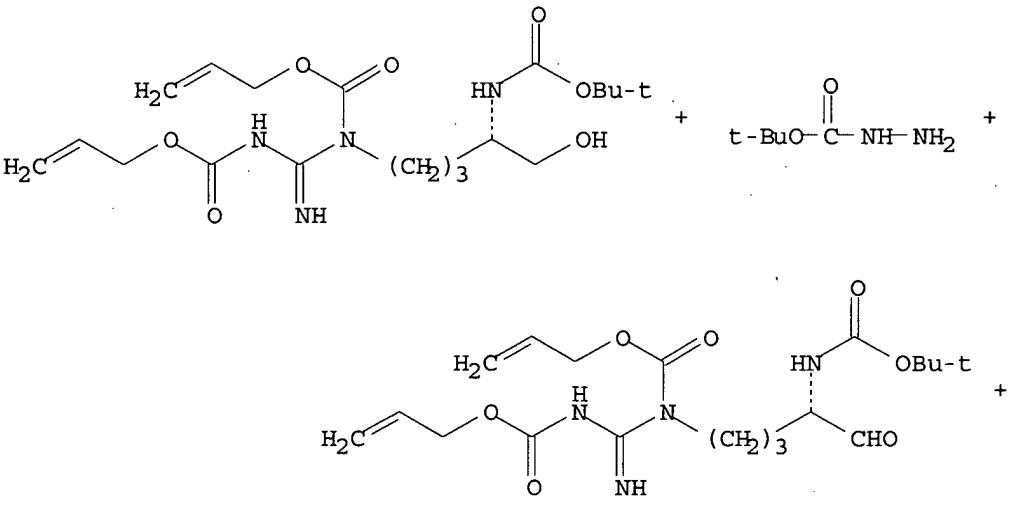
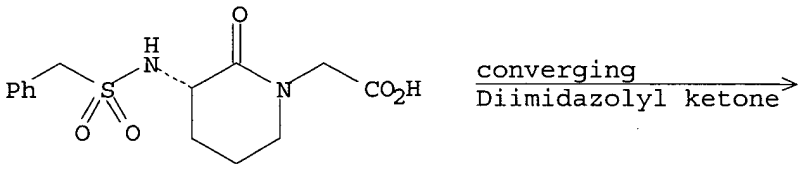
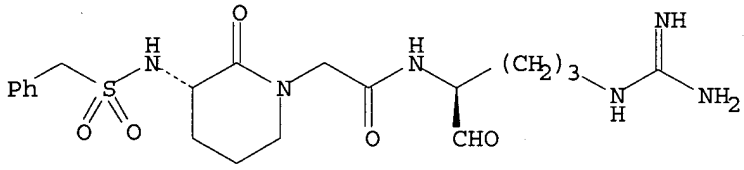
NOTE: RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, STEREOSELECTIVE

RX(210) OF 249 - 8 STEPS



RX(210) OF 249 - 8 STEPS





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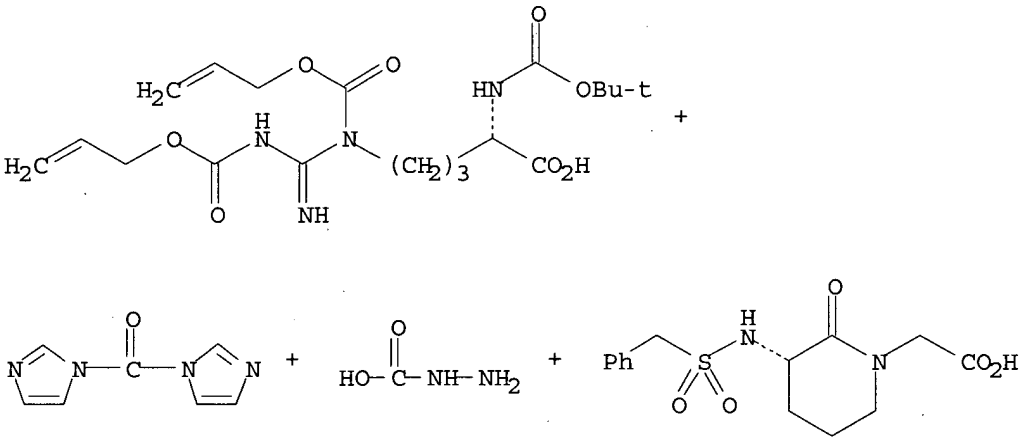
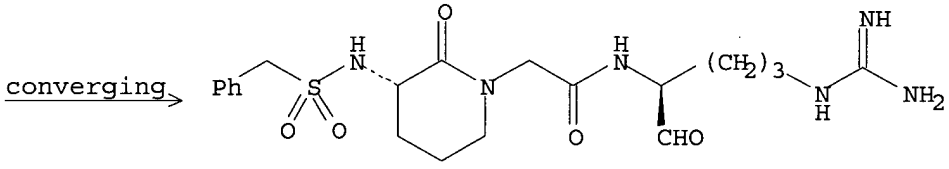
RX(212) OF 249 - 8 STEPS



RX(212) OF 249 - 8 STEPS



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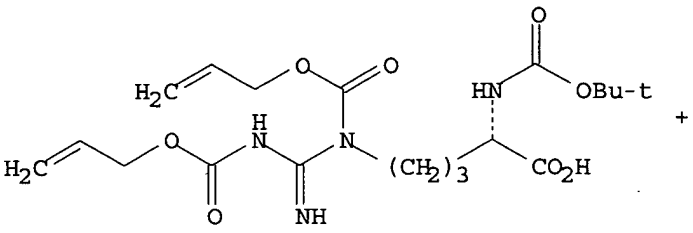
NOTE: STEREOSELECTIVE, STEREOSELECTIVE, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION

RX(214) OF 249 - 8 STEPS



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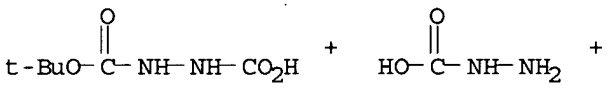

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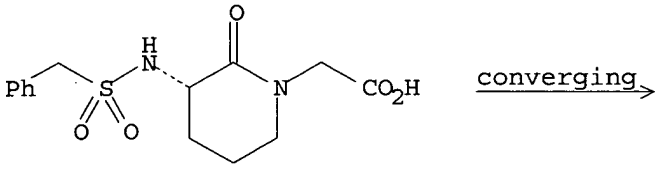
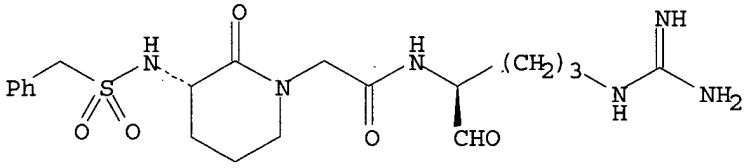


converging

RX(214) OF 249 - 8 STEPS



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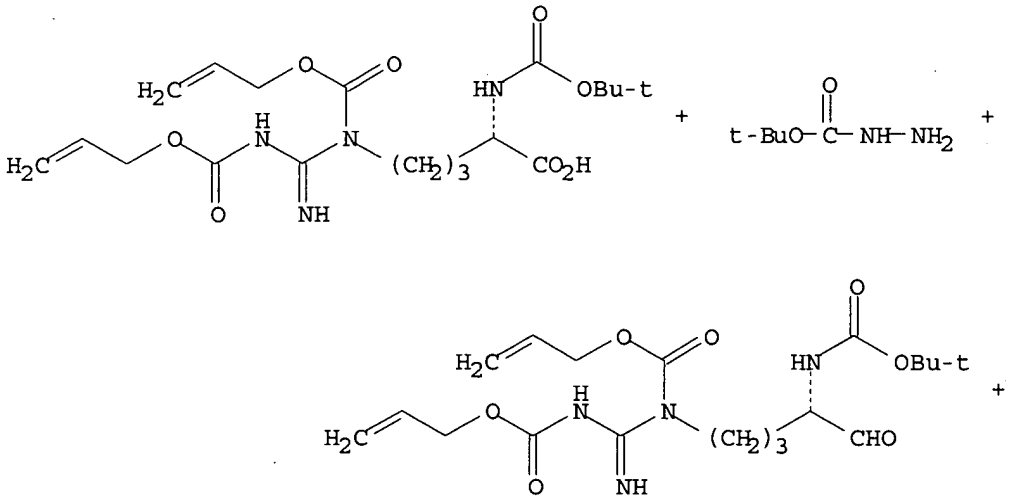
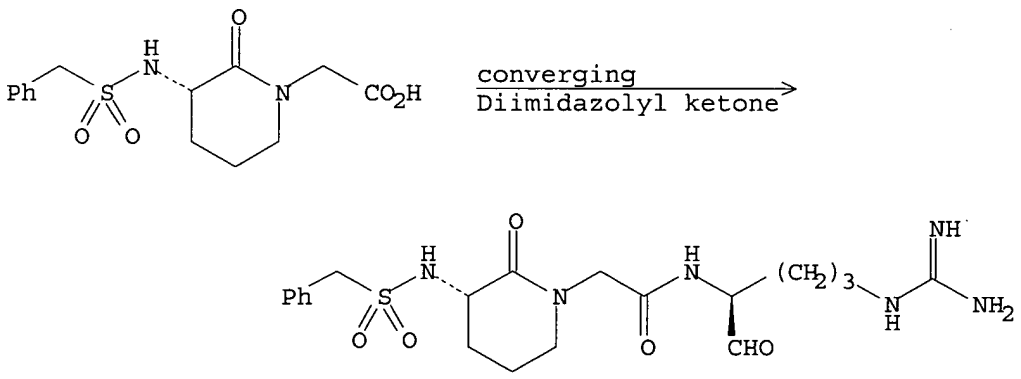
NOTE: STEREOSELECTIVE, STEREOSELECTIVE, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION

RX(224) OF 249 - 9 STEPS



RX(224) OF 249 - 9 STEPS



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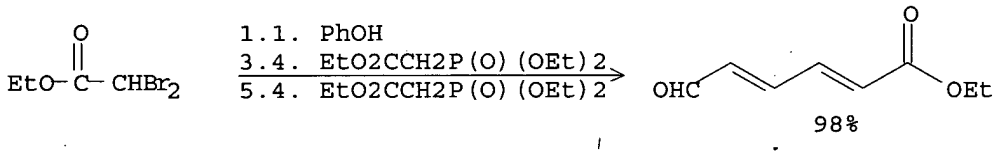
NOTE: RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, RESIN SUPPORTED REACTION, STEREOSELECTIVE, STEREOSELECTIVE

L13 ANSWER 4 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 132:12488 CASREACT
TITLE: Synthesis of isotopically labelled L-phenylalanine and L-tyrosine
AUTHOR(S): Raap, Jan; Nieuwenhuis, Saskia; Creemers, Alain; Hexspoor, Sander; Kragl, Udo; Lugtenburg, Johan
CORPORATE SOURCE: Institute Chemistry, Leiden Univ., Leiden, 2300 RA, Neth.
SOURCE: European Journal of Organic Chemistry (1999), (10), 2609-2621
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal
LANGUAGE: English

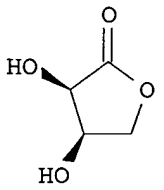
AB A synthetic route to stable-isotope-substituted L-phenylalanine is presented, which allows the introduction of 13C, 15N, and D labels at any position or combination of positions. For labeling of the aromatic ring, a synthetic route to PhCO2Et or PhCN was developed, based on the electrocyclic ring-closure of a 1,6-disubstituted hexatriene, with in-situ aromatization by elimination of 1 NH2 substituent. Several important, highly isotopically enriched synthons were prepared, namely PhCN, PhCHO, PhCO2Et, and (PhO)2CHCO2Et. Labeled L-phenylalanines were synthesized from both aromatic precursors by initial conversion into PhCH2COCO2Na and subsequent transformation into the L-α-amino acid by an enzymic reductive amination. In this manner, highly enriched phenylalanines are obtained on the 10-g scale and with ≥99% ee. The method was validated by the synthesis of [1'-13C]-L-Phe and [2-D]-L-Phe. Addnl., 2 methods are described for the introduction of isotopes into L-tyrosine starting from isotopically enriched PhCN and PhCO2Et.

RX(112) OF 162 - 6 STEPS

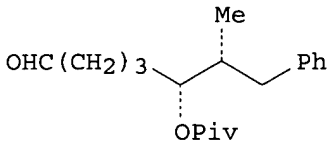


REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

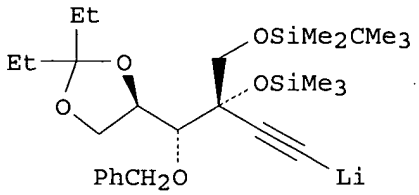
L13 ANSWER 5 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 123:56456 CASREACT
TITLE: Synthesis of (+)-Zaragozic Acid C
AUTHOR(S): Carreira, Erick M.; Du Bois, J.
CORPORATE SOURCE: Arnold and Mabel Beckman Laboratory for Chemical Synthesis, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Journal of the American Chemical Society (1994), 116(23), 10825-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



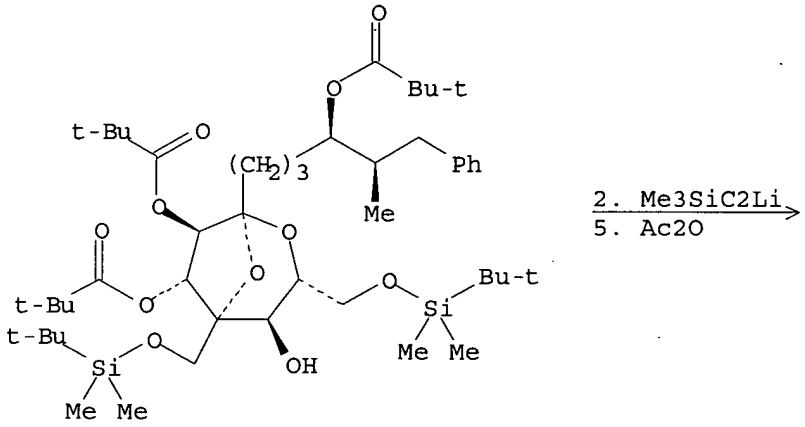
II



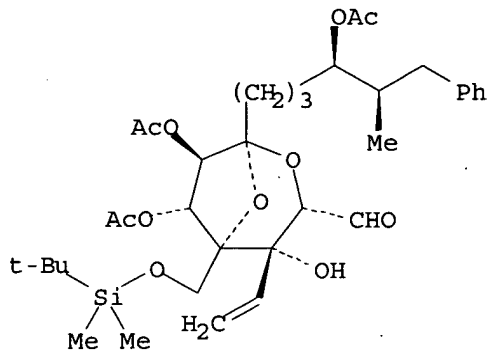
III

AB The asym. synthesis of the potent squalene synthetase inhibitor zaragozic acid C is described. The synthesis permits the preparation of multigram quantities of the dioxabicyclooctane core from the commercially available D-erythronic γ-lactone I. Coupling of the fully functionalized heptanal side chain II with lithium acetylide fragment III imparts convergency and flexibility to the synthesis.

RX(192) OF 473 - 8 STEPS



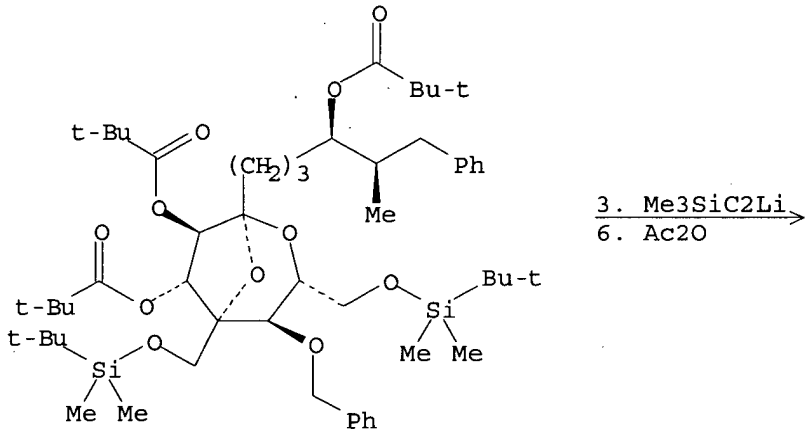
RX(192) OF 473 - 8 STEPS



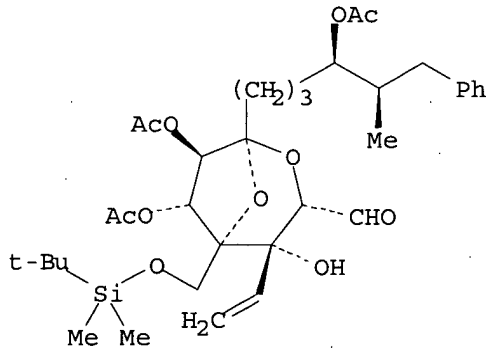
94%

NOTE: 1) Swern oxidn., in-situ generated reagent, 2) stereoselective, 6) regioselective, 7) chemoselective

RX(313) OF 473 - 9 STEPS



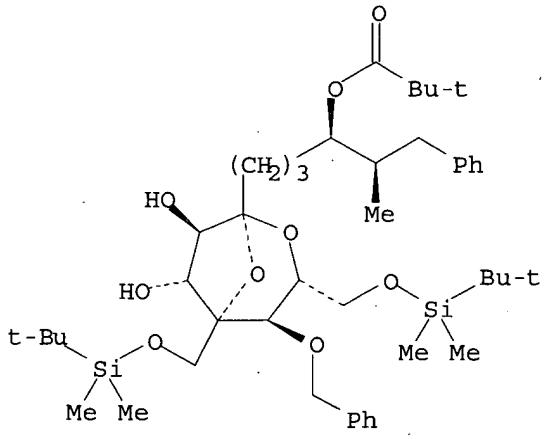
RX(313) OF 473 - 9 STEPS



94%

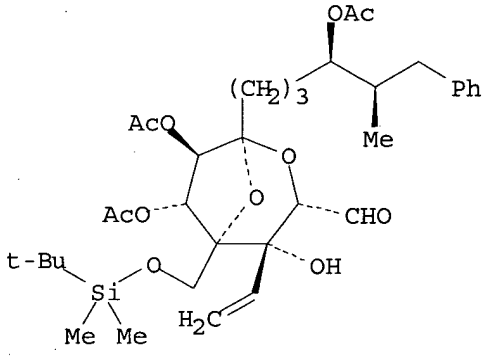
NOTE: 2) Swern oxidn., in-situ generated reagent, 3) stereoselective, 7) regioselective, 8) chemoselective

RX(314) OF 473 - 10 STEPS



1. Pivaloyl chloride
4. Me3SiC2Li
7. Ac2O

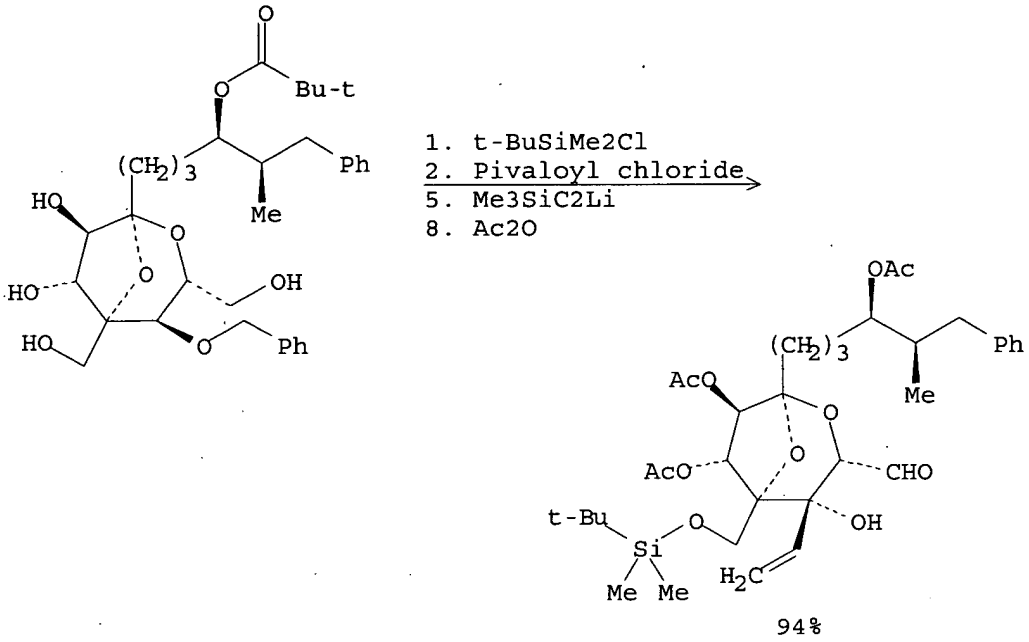
RX(314) OF 473 - 10 STEPS



94%

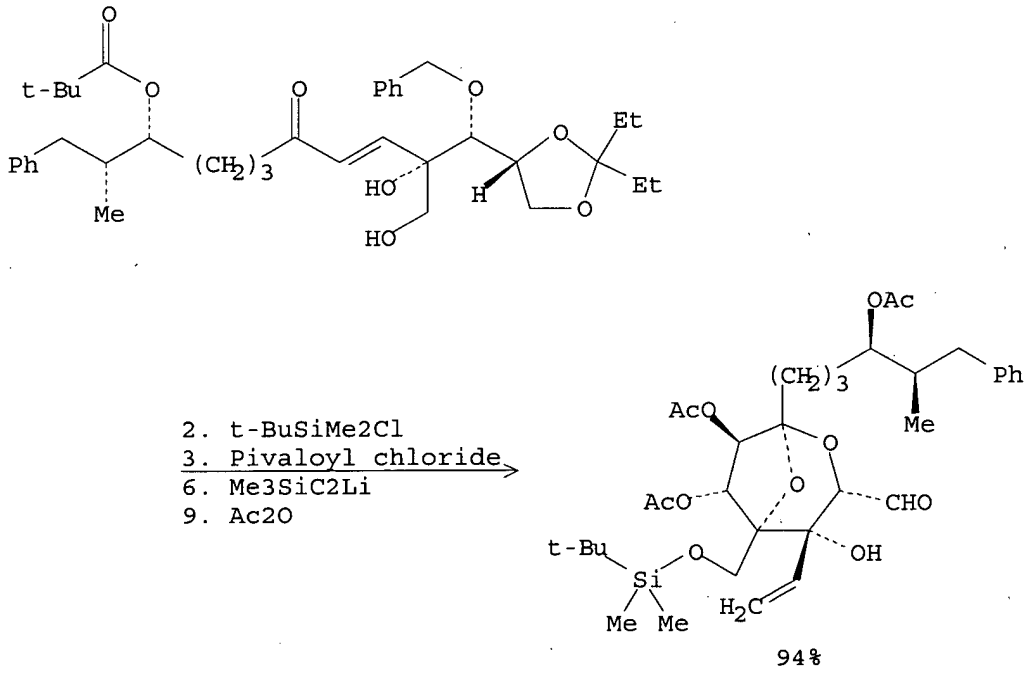
NOTE: 3) Swern oxidn., in-situ generated reagent, 4) stereoselective, 8) regioselective, 9) chemoselective

RX(315) OF 473 - 11 STEPS



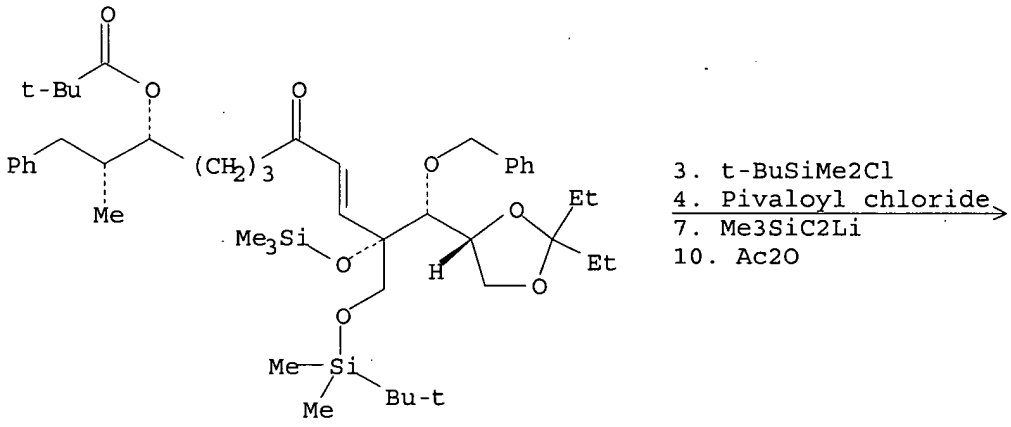
NOTE: 1) regioselective, 4) Swern oxidn., in-situ generated reagent,
5) stereoselective, 9) regioselective, 10) chemoselective

RX(316) OF 473 - 12 STEPS

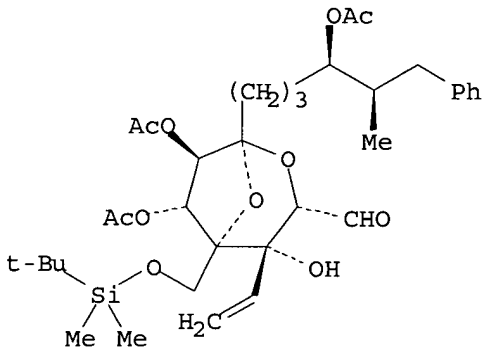


NOTE: 1) stereoselective, 2) regioselective, 5) Swern oxidn., in-situ generated reagent, 6) stereoselective, 10) regioselective, 11) chemoselective

RX(317) OF 473 - 13 STEPS



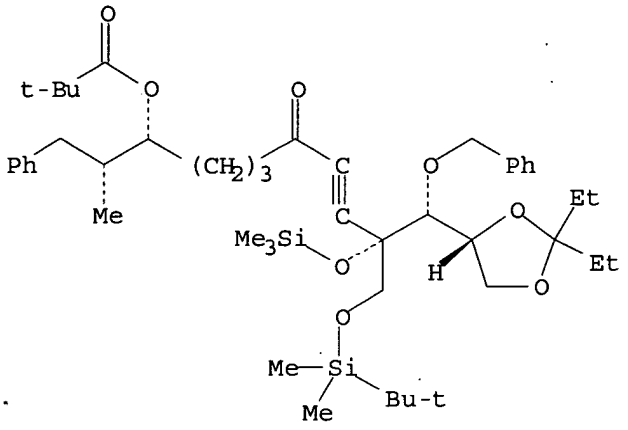
RX(317) OF 473 - 13 STEPS



94%

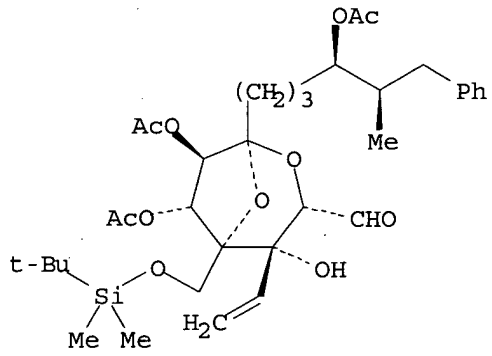
NOTE: 2) stereoselective, 3) regioselective, 6) Swern oxidn., in-situ generated reagent, 7) stereoselective, 11) regioselective, 12) chemoselective

RX(318) OF 473 - 14 STEPS



4. t-BuSiMe2Cl
5. Pivaloyl chloride
8. Me3SiC2Li
11. Ac2O

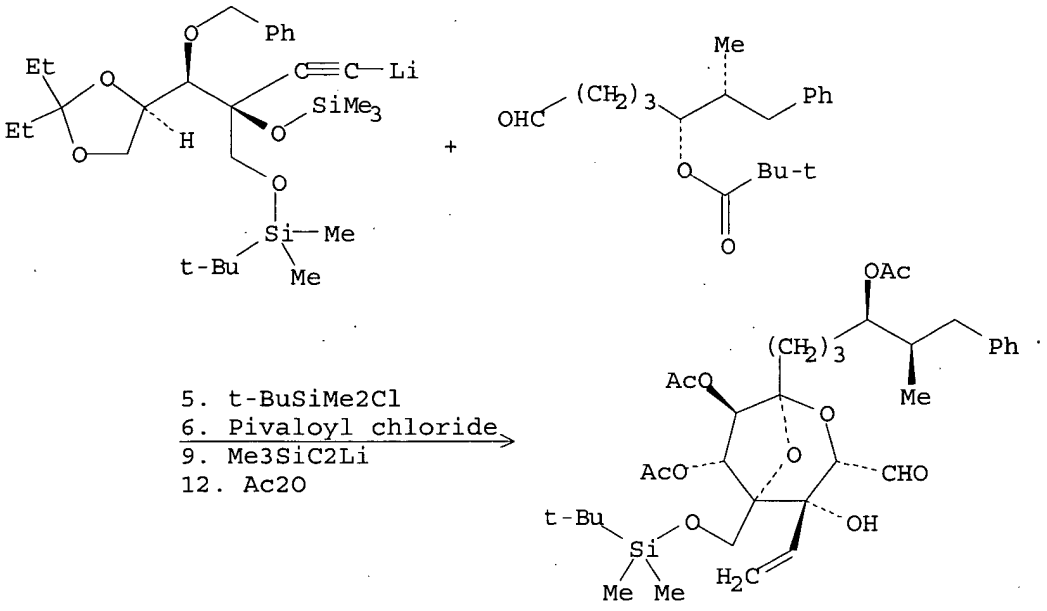
RX(318) OF 473 - 14 STEPS



94%

NOTE: 1) stereoselective, chemoselective, 3) stereoselective, 4) regioselective, 7) Swern oxidn., in-situ generated reagent, 8) stereoselective, 12) regioselective, 13) chemoselective

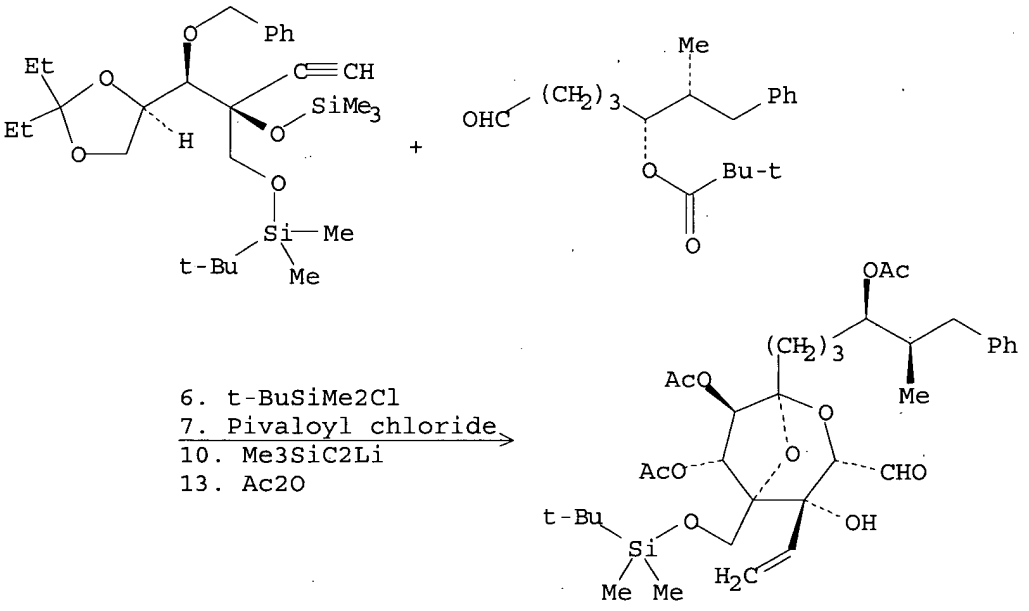
RX(319) OF 473 - 15 STEPS



94%

NOTE: 2) stereoselective, chemoselective, 4) stereoselective, 5) regioselective, 8) Swern oxidn., in-situ generated reagent, 9) stereoselective, 13) regioselective, 14) chemoselective

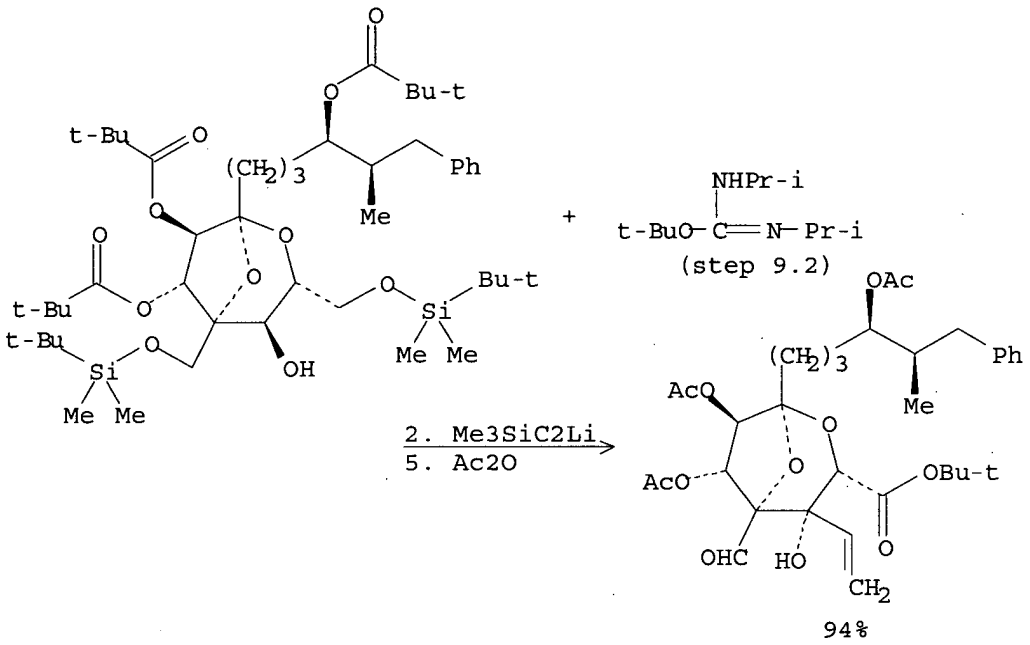
RX(320) OF 473 - 16 STEPS



94%

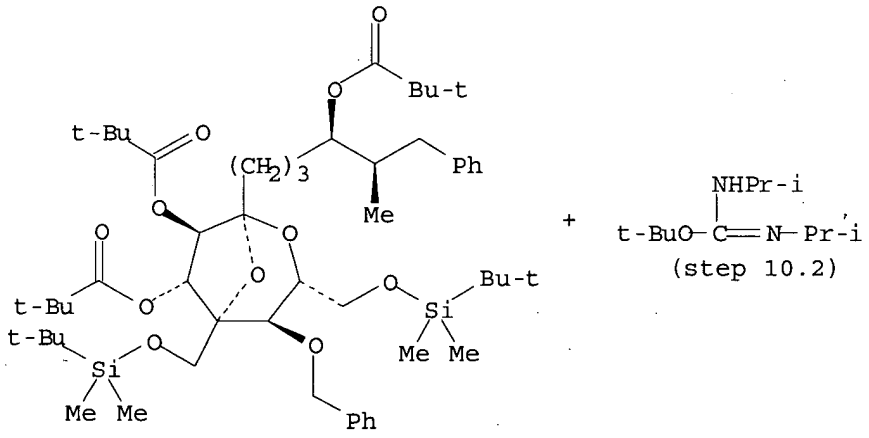
NOTE: 3) stereoselective, chemoselective, 5) stereoselective, 6) regioselective, 9) Swern oxidn., in-situ generated reagent, 10) stereoselective, 14) regioselective, 15) chemoselective

RX(339) OF 473 - 11 STEPS



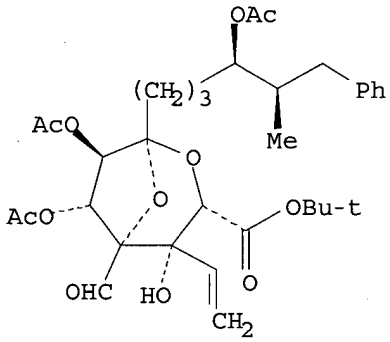
NOTE: 1) Swern oxidn., in-situ generated reagent, 2) stereoselective, 6) regioselective, 7) chemoselective, 9) buffered soln.

RX(340) OF 473 - 12 STEPS



3. Me3SiC2Li
6. Ac2O

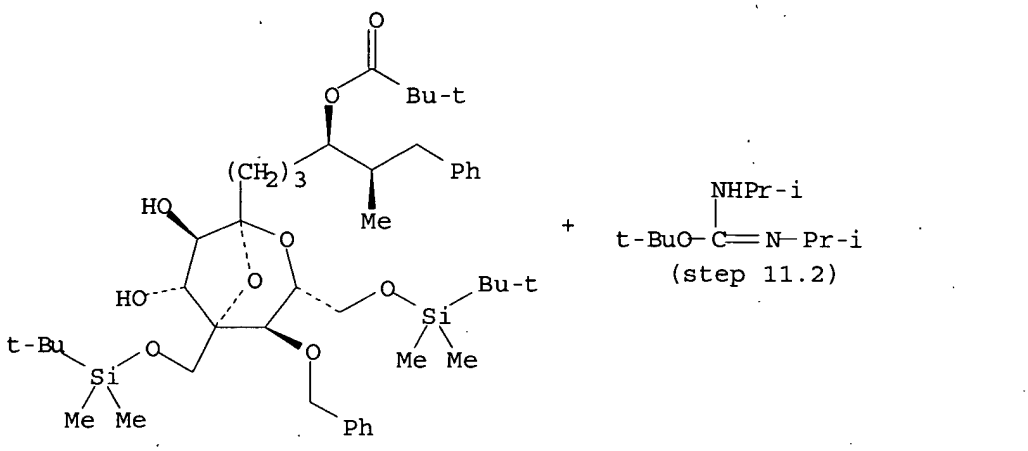
RX(340) OF 473 - 12 STEPS



94%

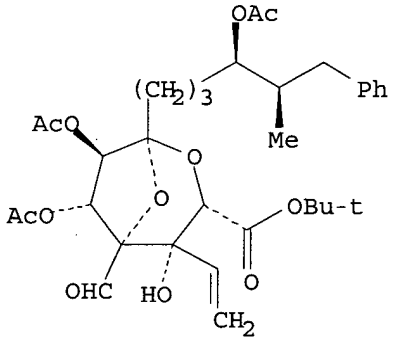
NOTE: 2) Swern oxidn., in-situ generated reagent, 3) stereoselective, 7) regioselective, 8) chemoselective, 10) buffered soln.

RX(341) OF 473 - 13 STEPS



1. Pivaloyl chloride
4. Me3SiC2Li
7. Ac2O

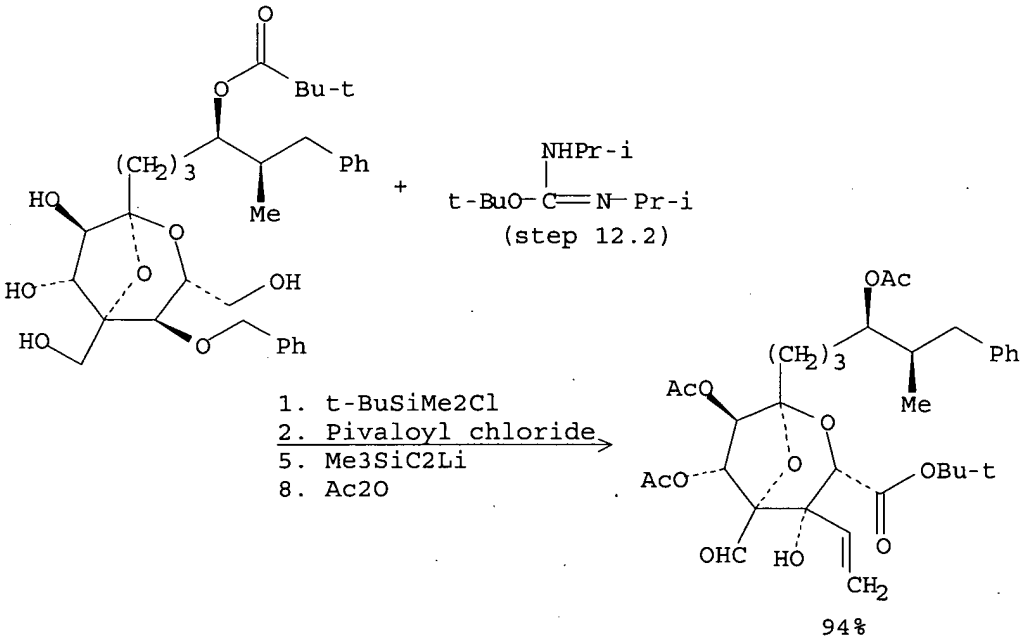
RX(341) OF 473 - 13 STEPS



94%

NOTE: 3) Swern oxidn., in-situ generated reagent, 4) stereoselective, 8) regioselective, 9) chemoselective, 11) buffered soln.

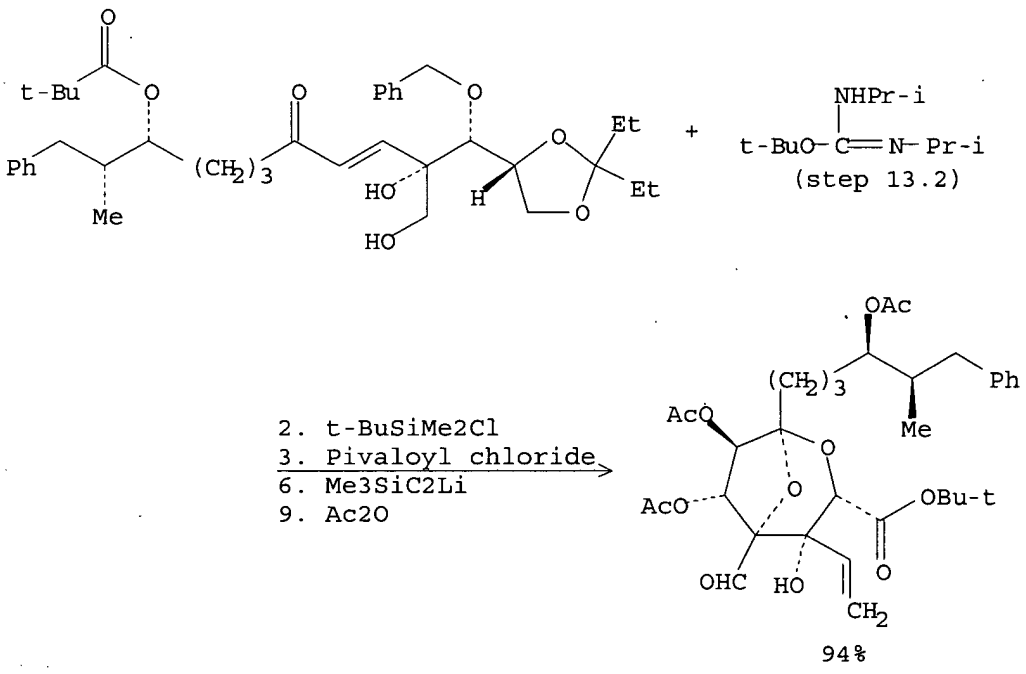
RX(342) OF 473 - 14 STEPS



94%

NOTE: 1) regioselective, 4) Swern oxidn., in-situ generated reagent, 5) stereoselective, 9) regioselective, 10) chemoselective, 12) buffered soln.

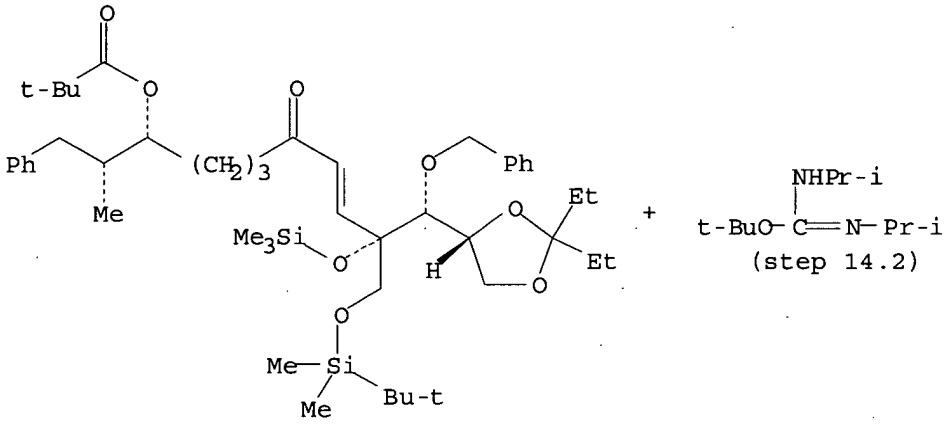
RX(343) OF 473 - 15 STEPS



94%

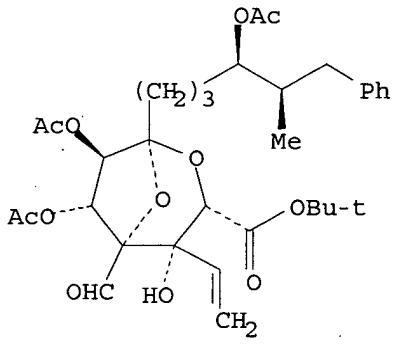
NOTE: 1) stereoselective, 2) regioselective, 5) Swern oxidn., in-situ generated reagent, 6) stereoselective, 10) regioselective, 11) chemoselective, 13) buffered soln.

RX(344) OF 473 - 16 STEPS



3. t-BuSiMe2Cl
4. Pivaloyl chloride
7. Me3SiC2Li
10. Ac2O

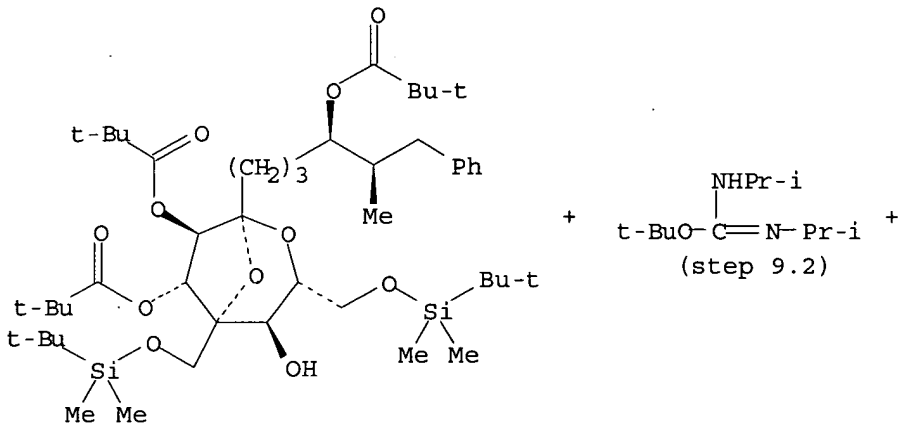
RX(344) OF 473 - 16 STEPS

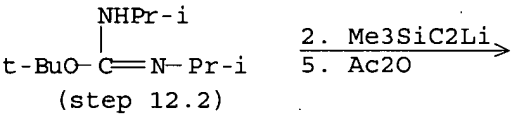


94%

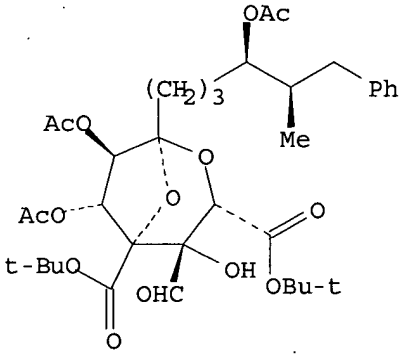
NOTE: 2) stereoselective, 3) regioselective, 6) Swern oxidn., in-situ generated reagent, 7) stereoselective, 11) regioselective, 12) chemoselective, 14) buffered soln.

RX(357) OF 473 - 13 STEPS





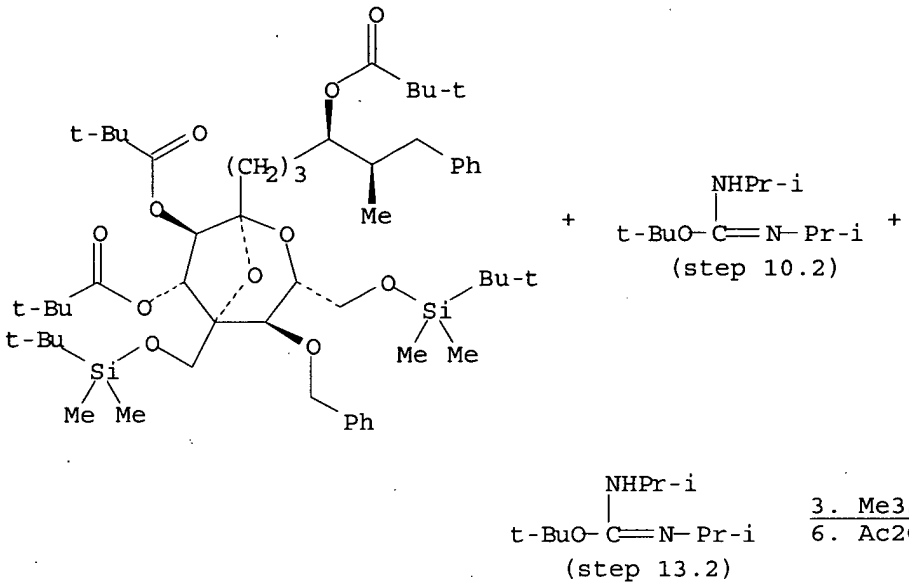
RX(357) OF 473 - 13 STEPS



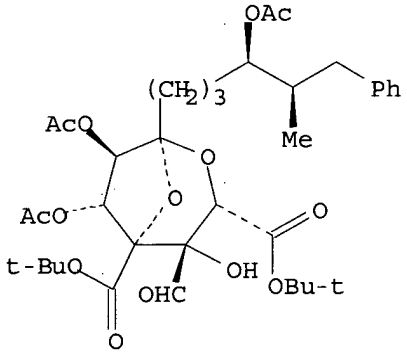
97%

NOTE: 1) Swern oxidn., in-situ generated reagent, 2) stereoselective, 6) regioselective, 7) chemoselective, 9) buffered soln., 12) buffered soln.

RX(358) OF 473 - 14 STEPS



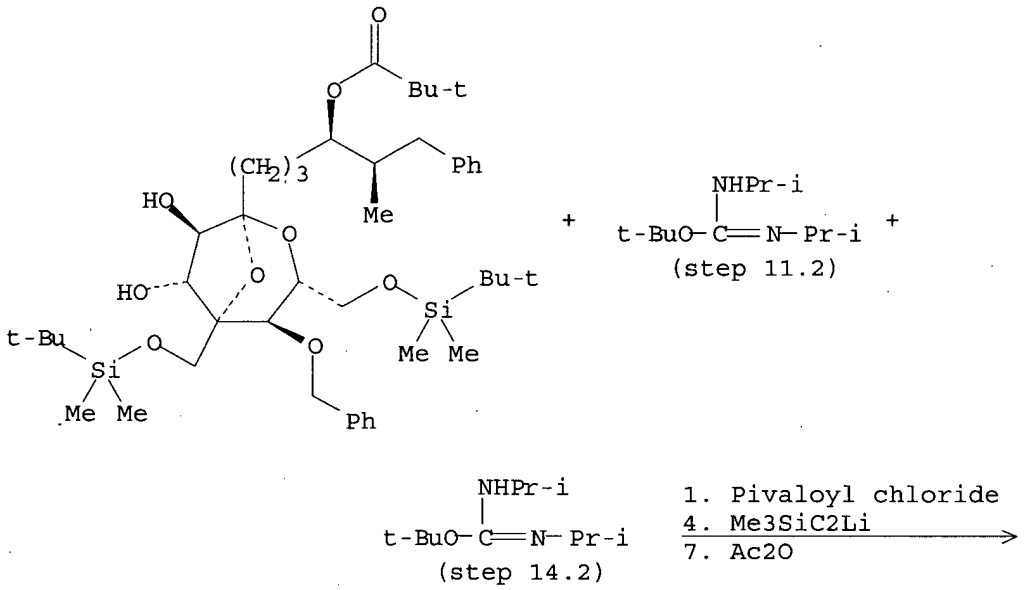
RX(358) OF 473 - 14 STEPS



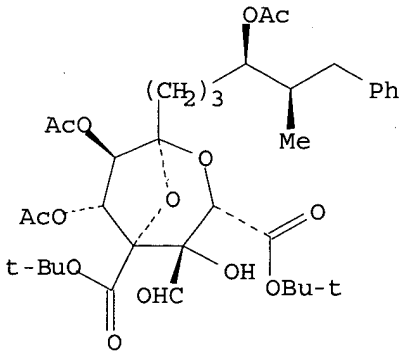
97%

NOTE: 2) Swern oxidn., in-situ generated reagent, 3) stereoselective, 7) regioselective, 8) chemoselective, 10) buffered soln., 13) buffered soln.

RX(359) OF 473 - 15 STEPS



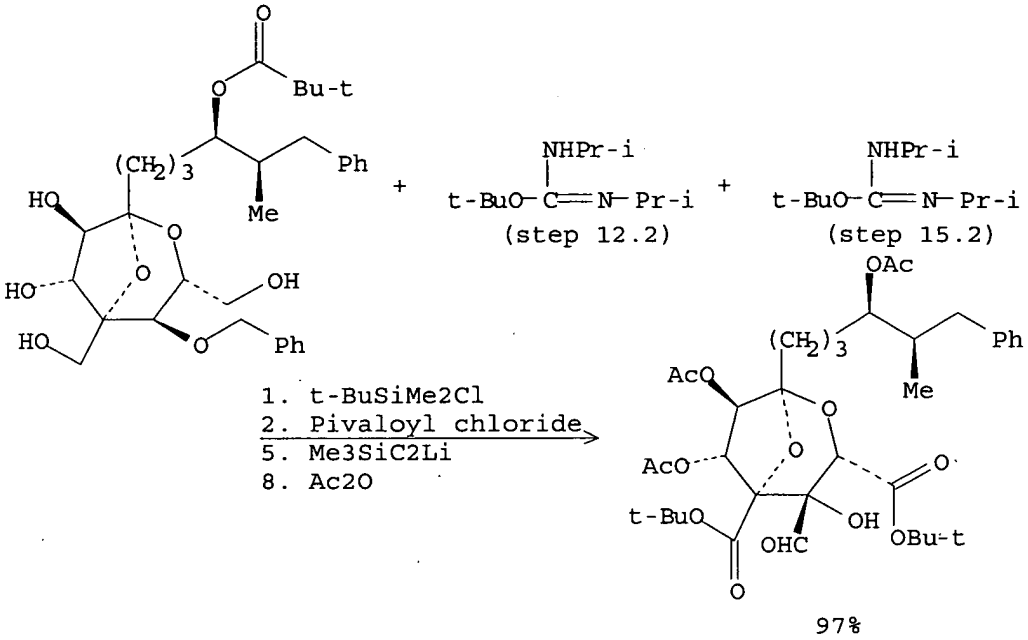
RX(359) OF 473 - 15 STEPS



97%

NOTE: 3) Swern oxidn., in-situ generated reagent, 4) stereoselective, 8) regioselective, 9) chemoselective, 11) buffered soln., 14) buffered soln.

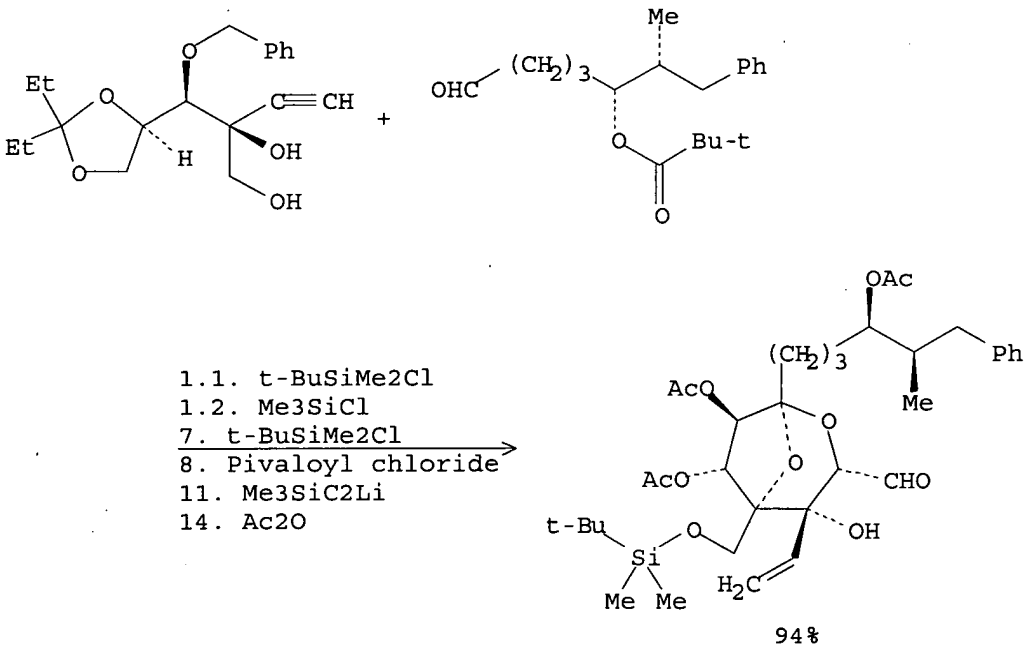
RX(360) OF 473 - 16 STEPS



97%

NOTE: 1) regioselective, 4) Swern oxidn., in-situ generated reagent, 5) stereoselective, 9) regioselective, 10) chemoselective, 12) buffered soln., 15) buffered soln.

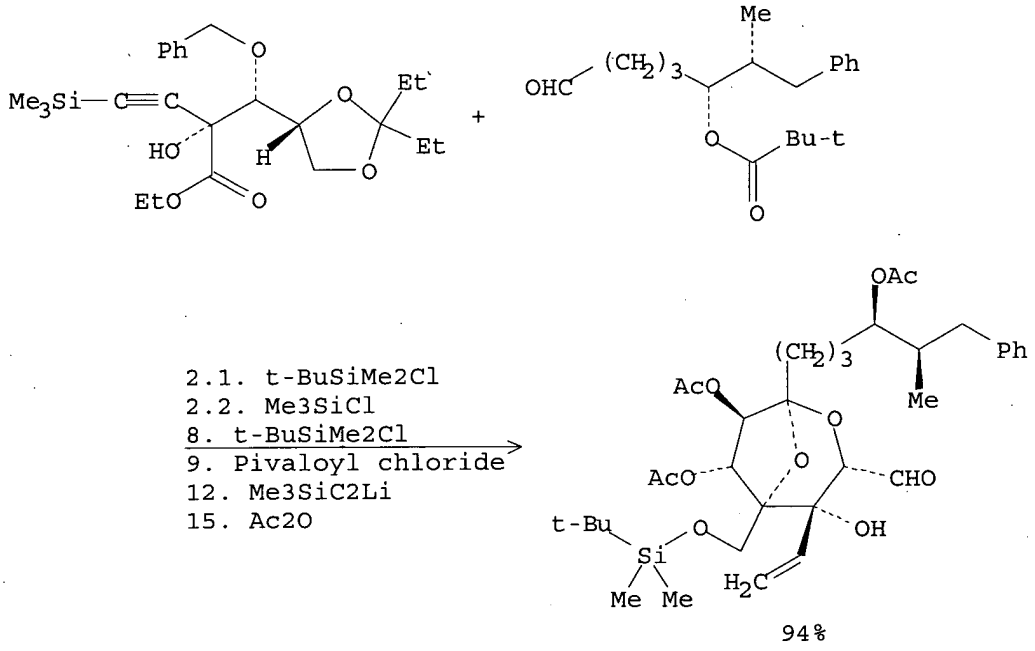
RX(414) OF 473 - 17 STEPS



94%

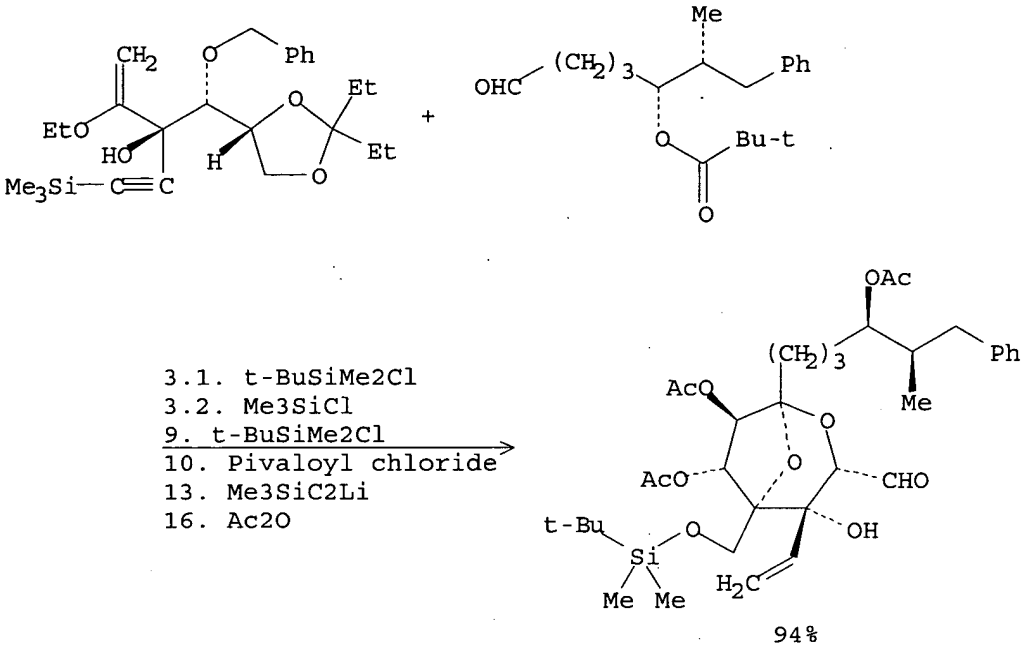
NOTE: 1) regioselective, scalable, 4) stereoselective, chemoselective, 6) stereoselective, 7) regioselective, 10) Swern oxidn., in-situ generated reagent, 11) stereoselective, 15) regioselective, 16) chemoselective

RX(415) OF 473 - 18 STEPS



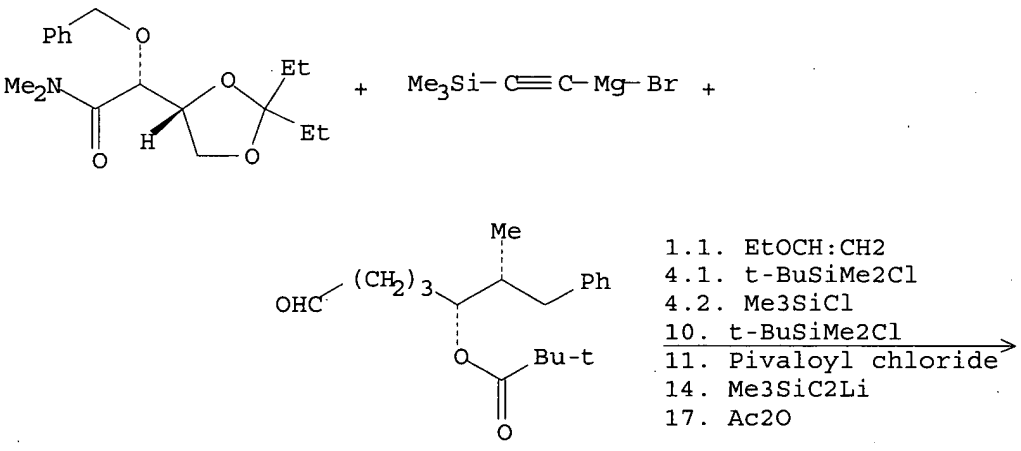
NOTE: 1) chemoselective (stage 1), 2) regioselective, scalable, 5) stereoselective, chemoselective, 7) stereoselective, 8) regioselective, 11) Swern oxidn., in-situ generated reagent, 12) stereoselective, 16) regioselective, 17) chemoselective

RX(416) OF 473 - 19 STEPS

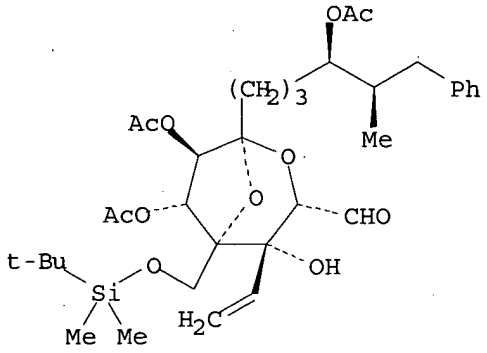


NOTE: 2) chemoselective (stage 1), 3) regioselective, scalable, 6) stereoselective, chemoselective, 8) stereoselective, 9) regioselective, 12) Swern oxidn., in-situ generated reagent, 13) stereoselective, 17) regioselective, 18) chemoselective

RX(417) OF 473 - 20 STEPS



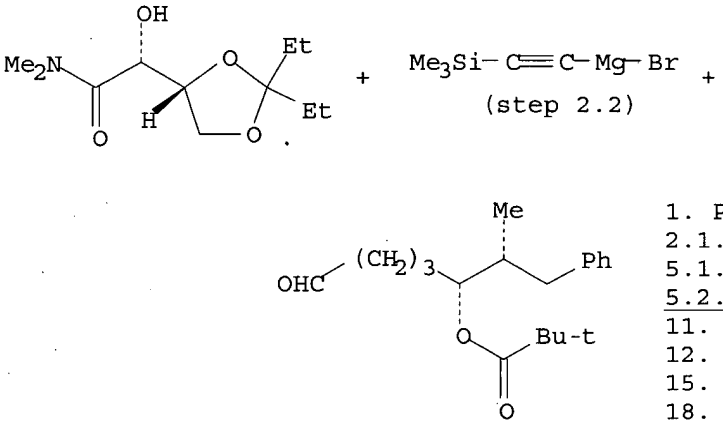
RX(417) OF 473 - 20 STEPS



94%

NOTE: 1) stereoselective, 3) chemoselective (stage 1), 4) regioselective, scalable, 7) stereoselective, chemoselective, 9) stereoselective, 10) regioselective, 13) Swern oxidn., in-situ generated reagent, 14) stereoselective, 18) regioselective, 19) chemoselective

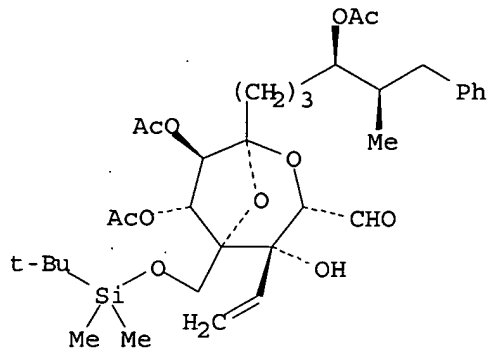
RX(418) OF 473 - 21 STEPS



(step 2.2)

1. PhCH2Cl
2.1. EtOCH:CH2
5.1. t-BuSiMe2Cl
5.2. Me3SiCl
11. t-BuSiMe2Cl
12. Pivaloyl chloride
15. Me3SiC2Li
18. Ac2O

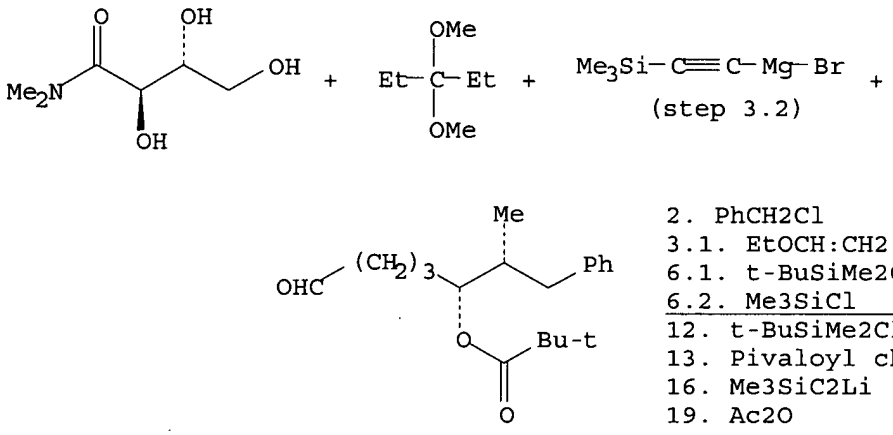
RX(418) OF 473 - 21 STEPS



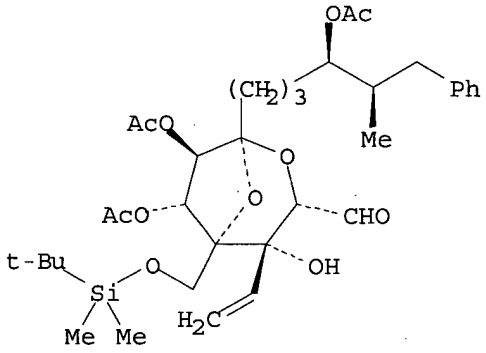
94%

NOTE: 2) stereoselective, 4) chemoselective (stage 1), 5) regioselective, scalable, 8) stereoselective, chemoselective, 10) stereoselective, 11) regioselective, 14) Swern oxidn., in-situ generated reagent, 15) stereoselective, 19) regioselective, 20) chemoselective

RX(419) OF 473 - 22 STEPS



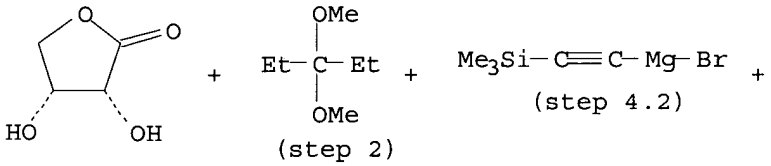
RX(419) OF 473 - 22 STEPS

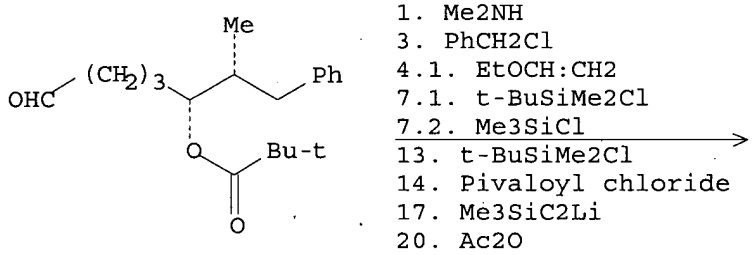


94%

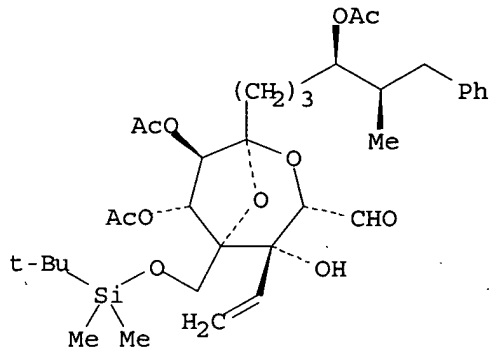
NOTE: 1) regioselective, acidic conditions, 3) stereoselective, 5) chemoselective (stage 1), 6) regioselective, scalable, 9) stereoselective, chemoselective, 11) stereoselective, 12) regioselective, 15) Swern oxidn., in-situ generated reagent, 16) stereoselective, 20) regioselective, 21) chemoselective

RX(420) OF 473 - 23 STEPS





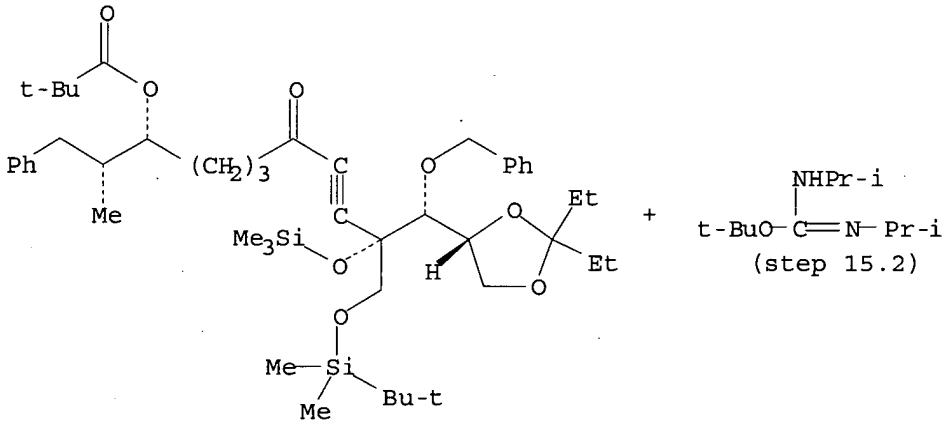
RX(420) OF 473 - 23 STEPS



94%

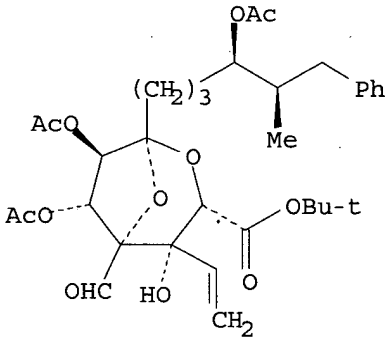
NOTE: 2) regioselective, acidic conditions, 4) stereoselective, 6) chemoselective (stage 1), 7) regioselective, scalable, 10) stereoselective, chemoselective, 12) stereoselective, 13) regioselective, 16) Swern oxidn., in-situ generated reagent, 17) stereoselective, 21) regioselective, 22) chemoselective

RX(438) OF 473 - 17 STEPS



4. t-BuSiMe2Cl
5. Pivaloyl chloride
8. Me3SiC2Li
11. Ac2O

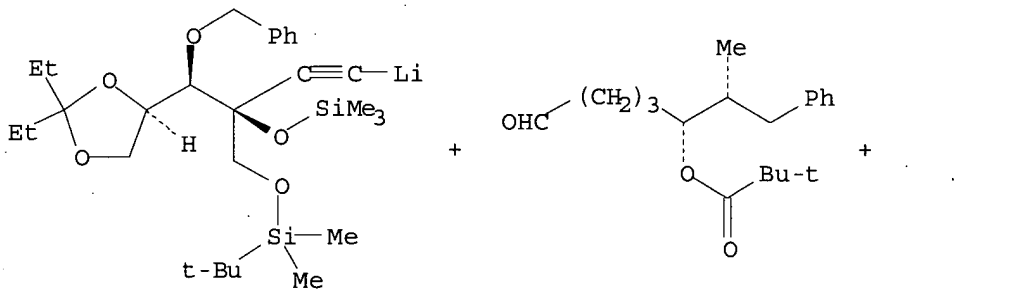
RX(438) OF 473 - 17 STEPS

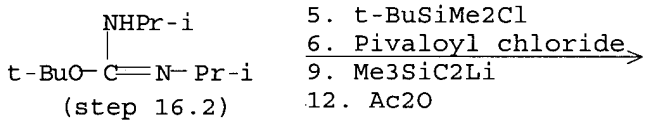


94%

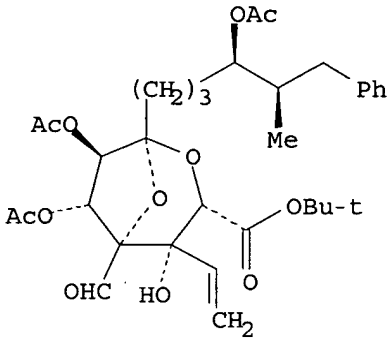
NOTE: 1) stereoselective, chemoselective, 3) stereoselective, 4) regioselective, 7) Swern oxidn., in-situ generated reagent, 8) stereoselective, 12) regioselective, 13) chemoselective, 15) buffered soln.

RX(439) OF 473 - 18 STEPS





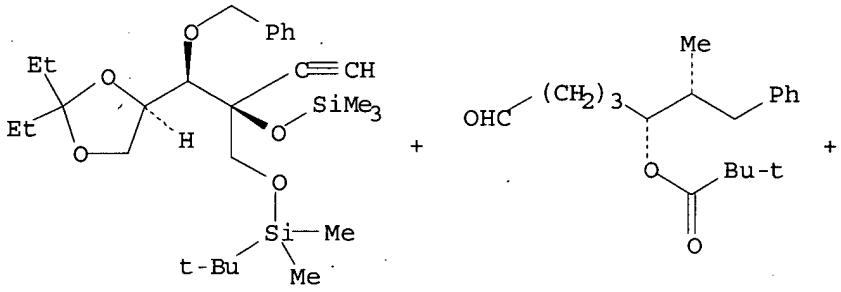
RX(439) OF 473 - 18 STEPS

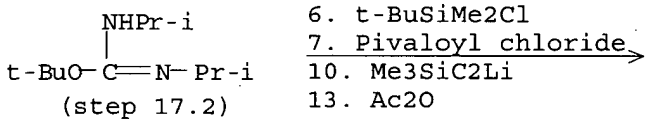


94%

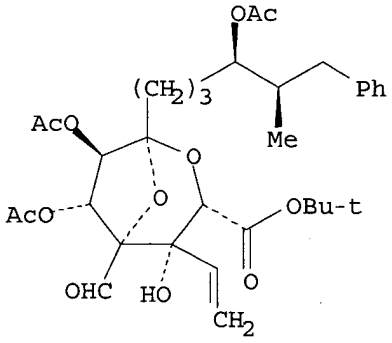
NOTE: 2) stereoselective, chemoselective, 4) stereoselective, 5) regioselective, 8) Swern oxidn., in-situ generated reagent, 9) stereoselective, 13) regioselective, 14) chemoselective, 16) buffered soln.

RX(440) OF 473 - 19 STEPS





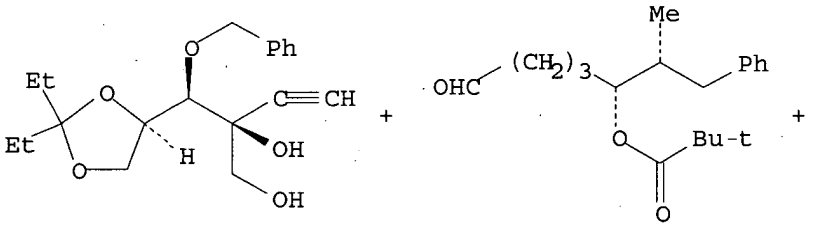
RX(440) OF 473 - 19 STEPS

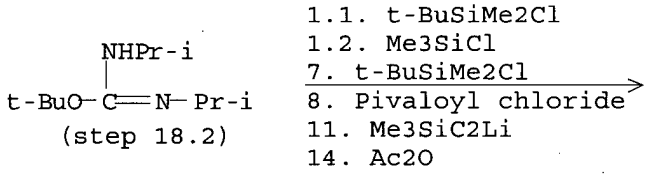


94%

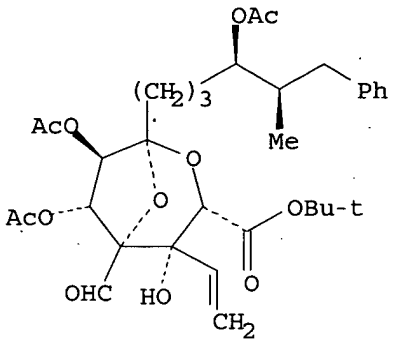
NOTE: 3) stereoselective, chemoselective, 5) stereoselective, 6) regioselective, 9) Swern oxidn., in-situ generated reagent, 10) stereoselective, 14) regioselective, 15) chemoselective, 17) buffered soln.

RX(441) OF 473 - 20 STEPS





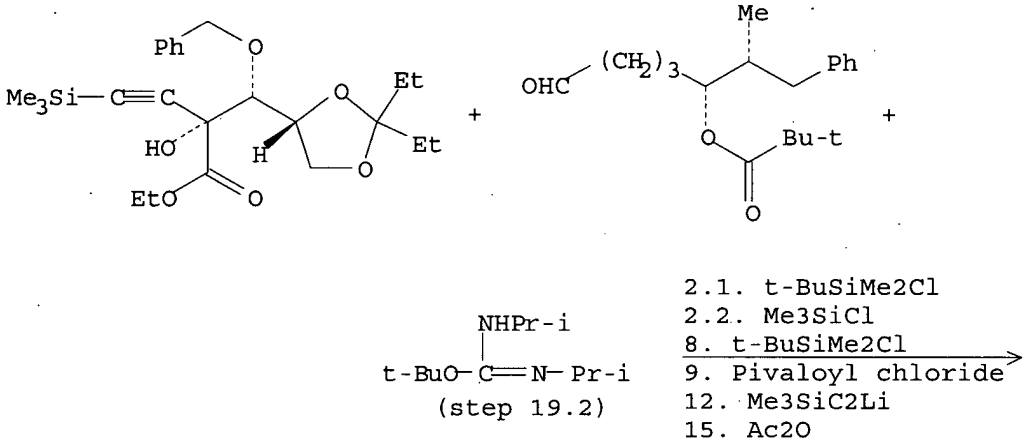
RX(441) OF 473 - 20 STEPS



94%

NOTE: 1) regioselective, scalable, 4) stereoselective, chemoselective, 6) stereoselective, 7) regioselective, 10) Swern oxidn., in-situ generated reagent, 11) stereoselective, 15) regioselective, 16) chemoselective, 18) buffered soln.

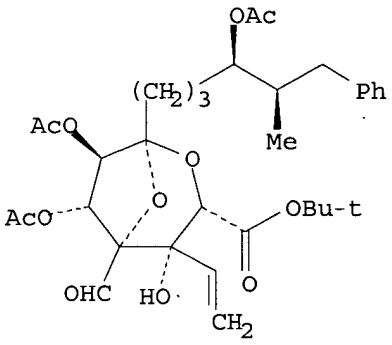
RX(442) OF 473 - 21 STEPS



2.1. t-BuSiMe2Cl
2.2. Me3SiCl
8. t-BuSiMe2Cl
9. Pivaloyl chloride
12. Me3SiC2Li
15. Ac2O

(step 19.2)

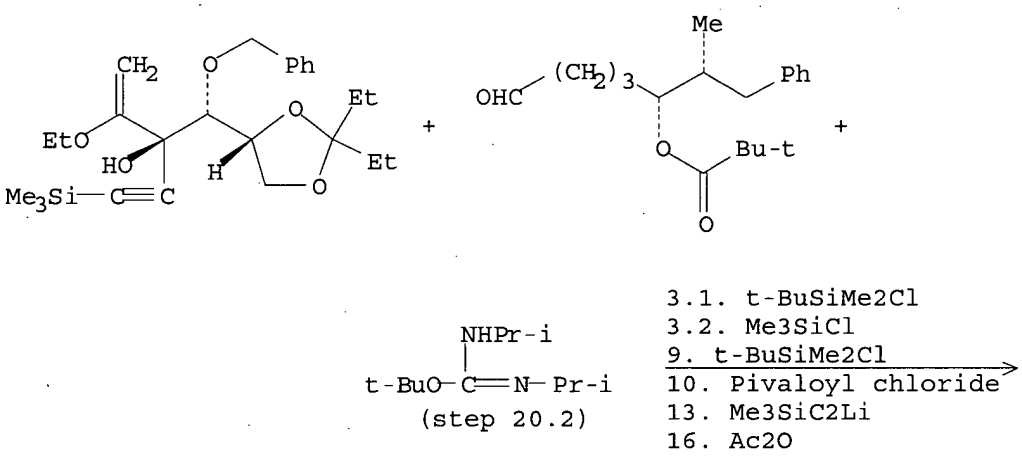
RX(442) OF 473 - 21 STEPS



94%

NOTE: 1) chemoselective (stage 1), 2) regioselective, scalable, 5) stereoselective, chemoselective, 7) stereoselective, 8) regioselective, 11) Swern oxidn., in-situ generated reagent, 12) stereoselective, 16) regioselective, 17) chemoselective, 19) buffered soln.

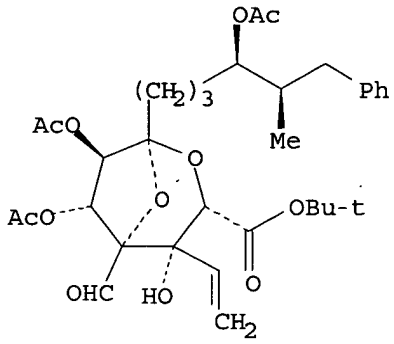
RX(443) OF 473 - 22 STEPS



3.1. t-BuSiMe2Cl
3.2. Me3SiCl
9. t-BuSiMe2Cl
10. Pivaloyl chloride
13. Me3SiC2Li
16. Ac2O

(step 20.2)

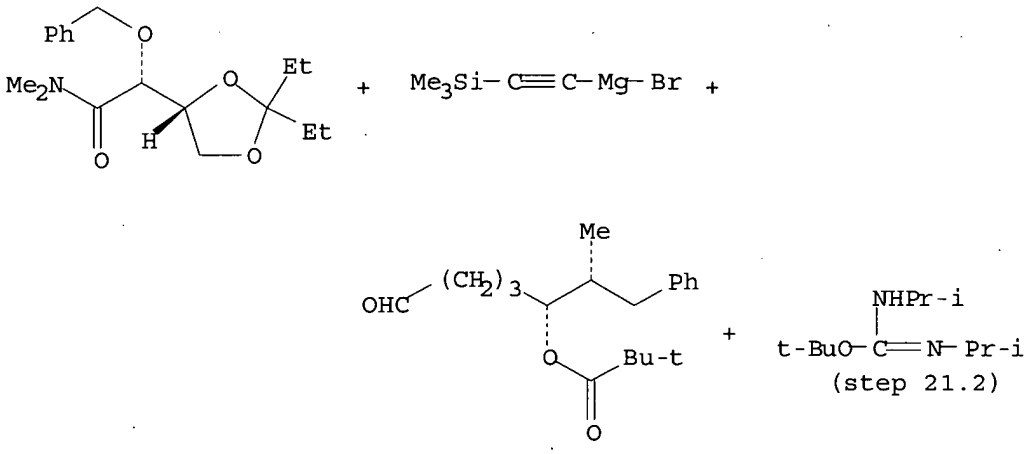
RX(443) OF 473 - 22 STEPS



94%

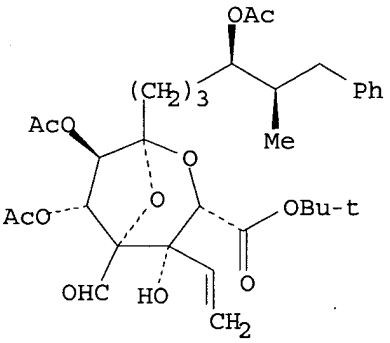
NOTE: 2) chemoselective (stage 1), 3) regioselective, scalable, 6) stereoselective, chemoselective, 8) stereoselective, 9) regioselective, 12) Swern oxidn., in-situ generated reagent, 13) stereoselective, 17) regioselective, 18) chemoselective, 20) buffered soln.

RX(444) OF 473 - 23 STEPS



RX(444) OF 473 - 23 STEPS

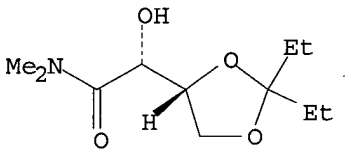
1.1. EtOCH:CH2
4.1. t-BuSiMe2Cl
4.2. Me3SiCl
10. t-BuSiMe2Cl
11. Pivaloyl chloride
14. Me3SiC2Li
17. Ac2O



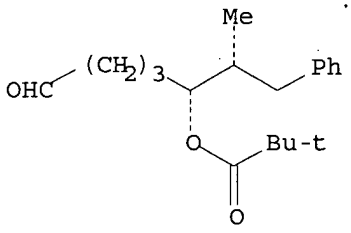
94%

NOTE: 1) stereoselective, 3) chemoselective (stage 1), 4) regioselective, scalable, 7) stereoselective, chemoselective, 9) stereoselective, 10) regioselective, 13) Swern oxidn., in-situ generated reagent, 14) stereoselective, 18) regioselective, 19) chemoselective, 21) buffered soln.

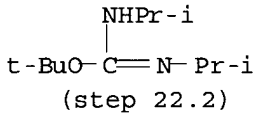
RX(445) OF 473 - 24 STEPS



+ $Me_3Si-C\equiv C-Mg-Br$ (step 2.2) +



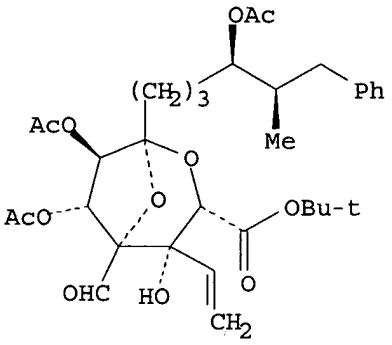
+



(step 22.2)

RX(445) OF 473 - 24 STEPS

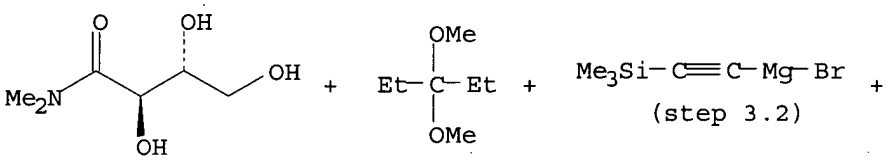
1. PhCH2Cl
2.1. EtOCH:CH2
5.1. t-BuSiMe2Cl
5.2. Me3SiCl
11. t-BuSiMe2Cl
12. Pivaloyl chloride
15. Me3SiC2Li
18. Ac2O



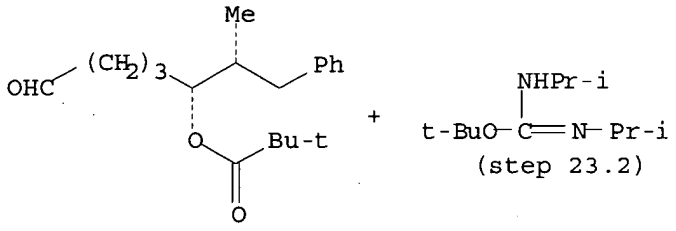
94%

NOTE: 2) stereoselective, 4) chemoselective (stage 1), 5) regioselective, scalable, 8) stereoselective, chemoselective, 10) stereoselective, 11) regioselective, 14) Swern oxidn., in-situ generated reagent, 15) stereoselective, 19) regioselective, 20) chemoselective, 22) buffered soln.

RX(446) OF 473 - 25 STEPS



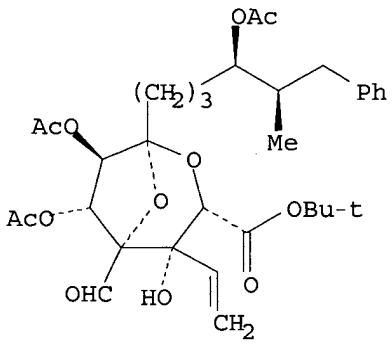
(step 3.2)



(step 23.2)

RX(446) OF 473 - 25 STEPS

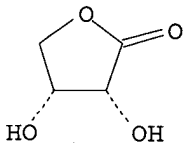
2. PhCH2Cl
3.1. EtOCH:CH2
6.1. t-BuSiMe2Cl
6.2. Me3SiCl
12. t-BuSiMe2Cl
13. Pivaloyl chloride
16. Me3SiC2Li
19. Ac2O



94%

NOTE: 1) regioselective, acidic conditions, 3) stereoselective, 5) chemoselective (stage 1), 6) regioselective, scalable, 9) stereoselective, chemoselective, 11) stereoselective, 12) regioselective, 15) Swern oxidn., in-situ generated reagent, 16) stereoselective, 20) regioselective, 21) chemoselective, 23) buffered soln.

RX(447) OF 473 - 26 STEPS



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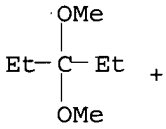
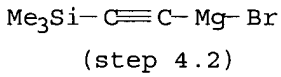


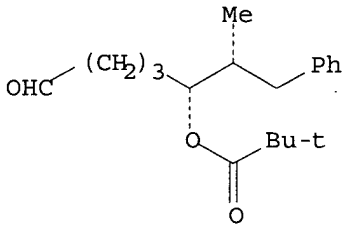
(step 2)

+



(step 4.2)

+



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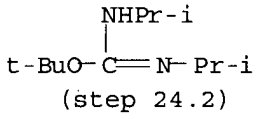
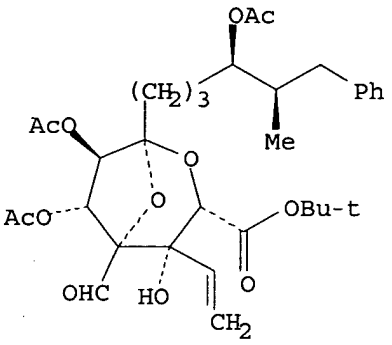


(step 24.2)

RX(447) OF 473 - 26 STEPS

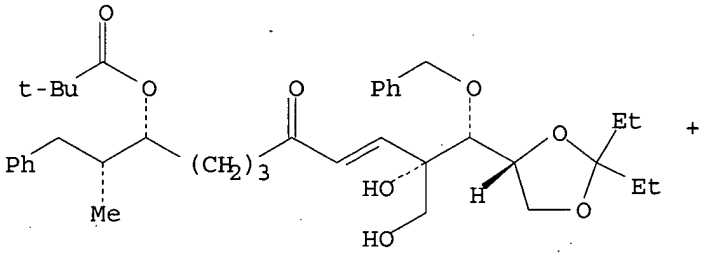
1. Me2NH
3. PhCH2Cl
4.1. EtOCH:CH2
7.1. t-BuSiMe2Cl
7.2. Me3SiCl
13. t-BuSiMe2Cl
14. Pivaloyl chloride
17. Me3SiC2Li
20. Ac2O



94%

NOTE: 2) regioselective, acidic conditions, 4) stereoselective, 6) chemoselective (stage 1), 7) regioselective, scalable, 10) stereoselective, chemoselective, 12) stereoselective, 13) regioselective, 16) Swern oxidn., in-situ generated reagent, 17) stereoselective, 21) regioselective, 22) chemoselective, 24) buffered soln.

RX(459) OF 473 - 17 STEPS



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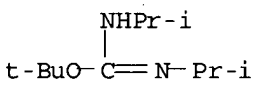
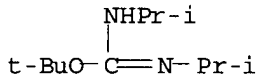


(step 13.2)

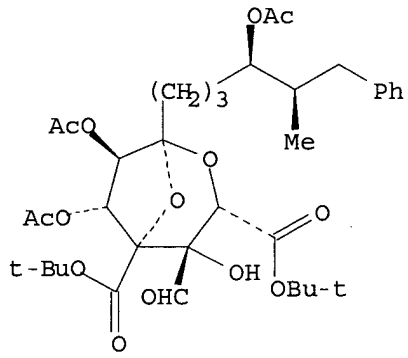
+



(step 16.2)

2. t-BuSiMe2Cl
3. Pivaloyl chloride
6. Me3SiC2Li
9. Ac2O

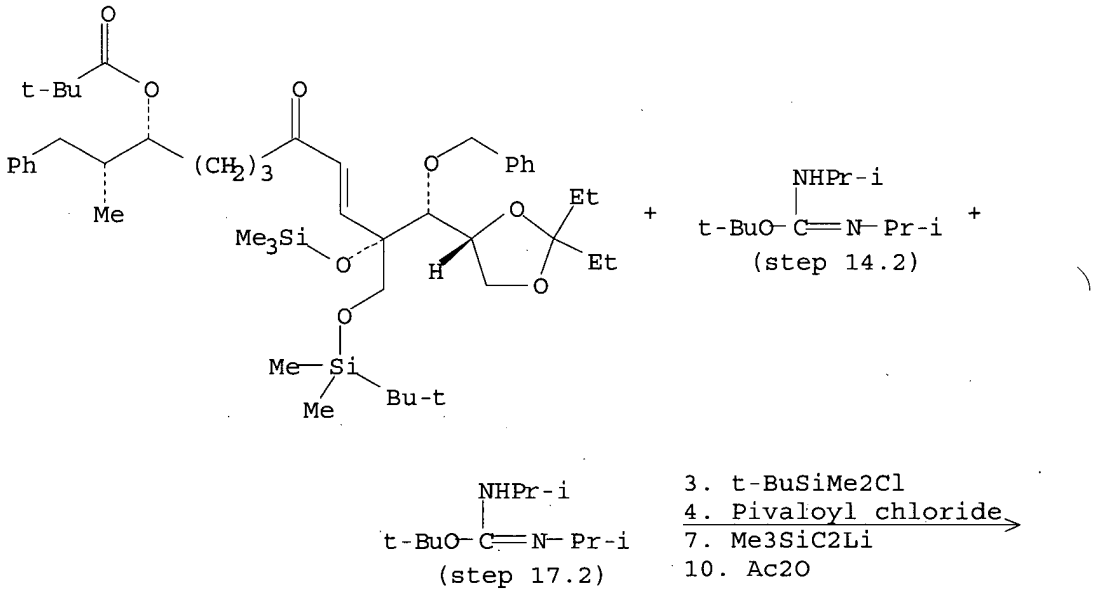
RX(459) OF 473 - 17 STEPS



97%

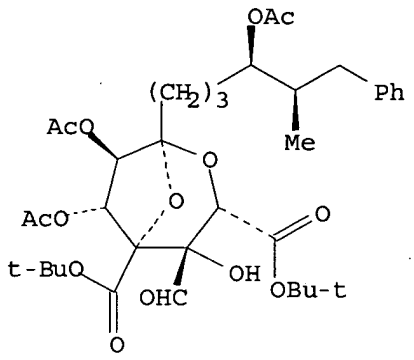
NOTE: 1) stereoselective, 2) regioselective, 5) Swern oxidn., in-situ generated reagent, 6) stereoselective, 10) regioselective, 11) chemoselective, 13) buffered soln., 16) buffered soln.

RX(460) OF 473 - 18 STEPS



3. t-BuSiMe2Cl
4. Pivaloyl chloride
7. Me3SiC2Li
10. Ac2O

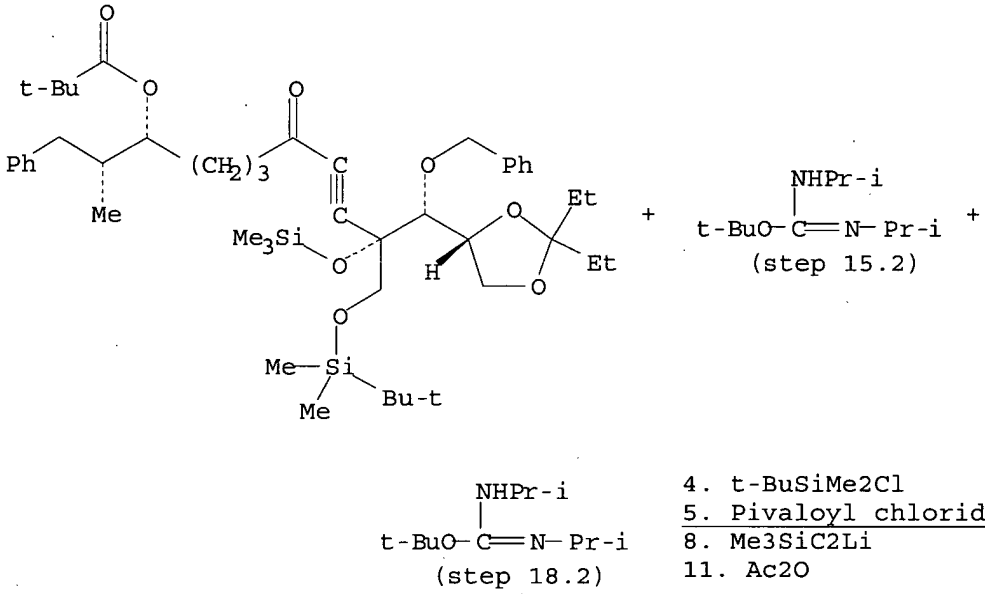
RX(460) OF 473 - 18 STEPS



97%

NOTE: 2) stereoselective, 3) regioselective, 6) Swern oxidn., in-situ generated reagent, 7) stereoselective, 11) regioselective, 12) chemoselective, 14) buffered soln., 17) buffered soln.

RX(461) OF 473 - 19 STEPS

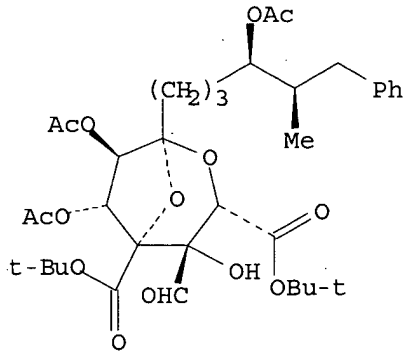


(step 15.2)

(step 18.2)

4. t-BuSiMe2Cl
5. Pivaloyl chloride
8. Me3SiC2Li
11. Ac2O

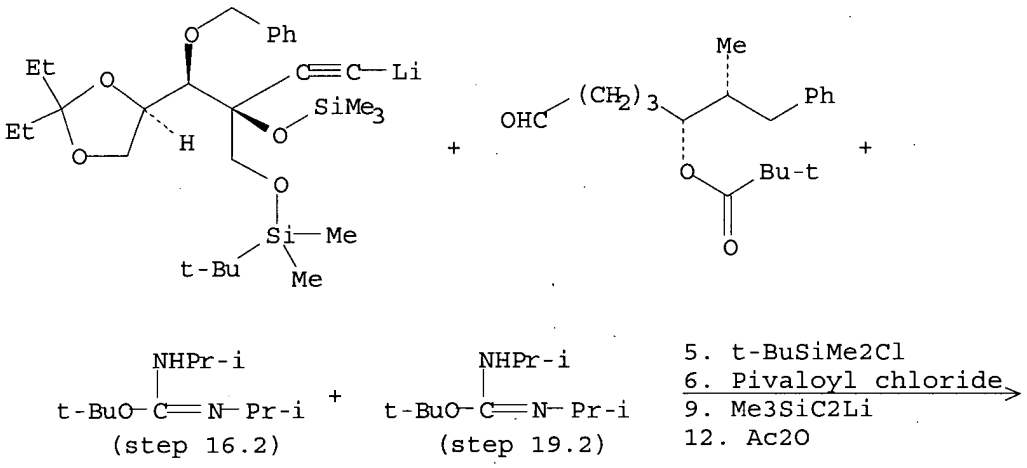
RX(461) OF 473 - 19 STEPS



97%

NOTE: 1) stereoselective, chemoselective, 3) stereoselective, 4) regioselective, 7) Swern oxidn., in-situ generated reagent, 8) stereoselective, 12) regioselective, 13) chemoselective, 15) buffered soln., 18) buffered soln.

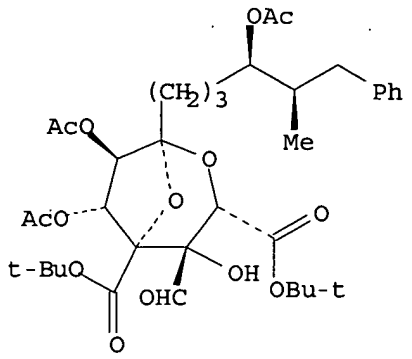
RX(462) OF 473 - 20 STEPS



(step 16.2) + (step 19.2)

5. t-BuSiMe2Cl
6. Pivaloyl chloride
9. Me3SiC2Li
12. Ac2O

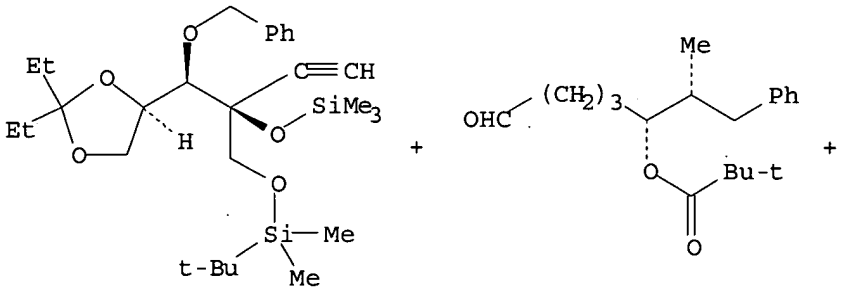
RX(462) OF 473 - 20 STEPS

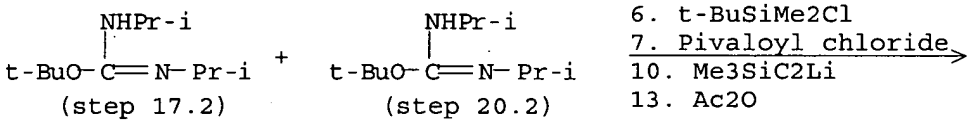


97%

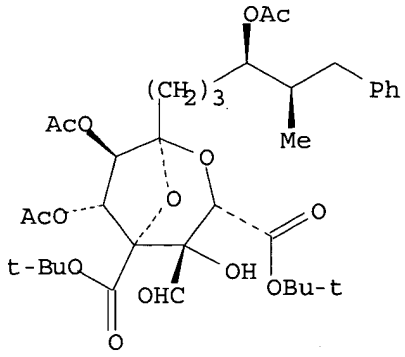
NOTE: 2) stereoselective, chemoselective, 4) stereoselective, 5) regioselective, 8) Swern oxidn., in-situ generated reagent, 9) stereoselective, 13) regioselective, 14) chemoselective, 16) buffered soln., 19) buffered soln.

RX(463) OF 473 - 21 STEPS





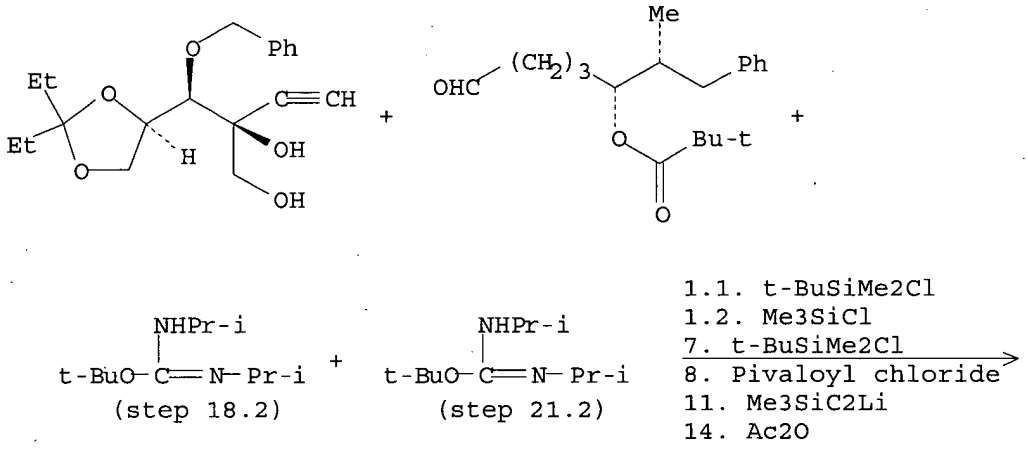
RX(463) OF 473 - 21 STEPS



97%

NOTE: 3) stereoselective, chemoselective, 5) stereoselective, 6) regioselective, 9) Swern oxidn., in-situ generated reagent, 10) stereoselective, 14) regioselective, 15) chemoselective, 17) buffered soln., 20) buffered soln.

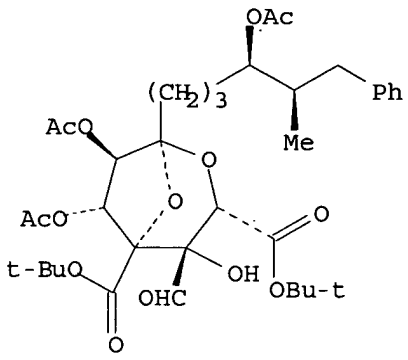
RX(464) OF 473 - 22 STEPS



1.1. t-BuSiMe2Cl
1.2. Me3SiCl
7. t-BuSiMe2Cl
8. Pivaloyl chloride
11. Me3SiC2Li
14. Ac2O

(step 18.2) (step 21.2)

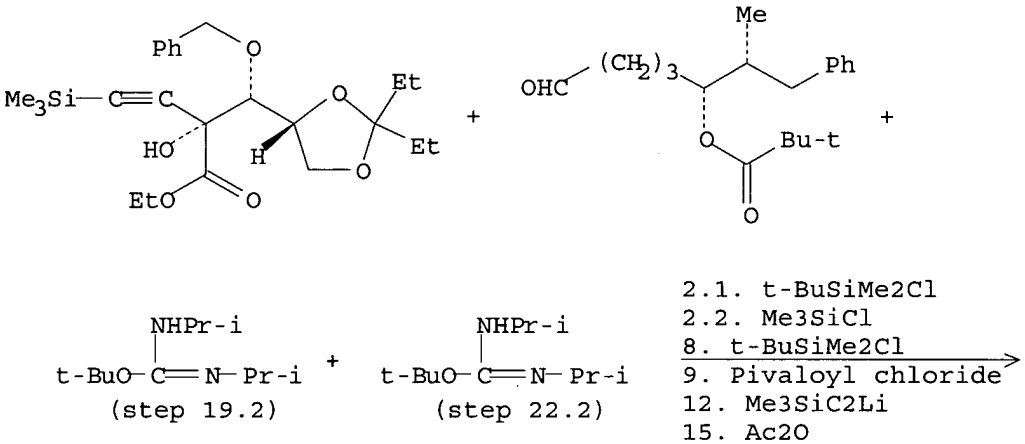
RX(464) OF 473 - 22 STEPS



97%

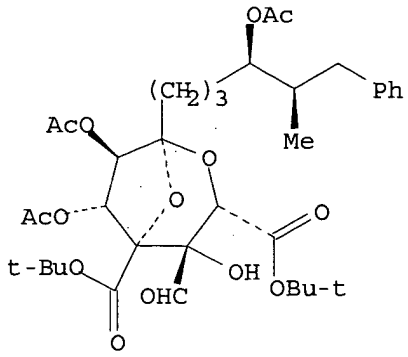
NOTE: 1) regioselective, scalable, 4) stereoselective, chemoselective, 6) stereoselective, 7) regioselective, 10) Swern oxidn., in-situ generated reagent, 11) stereoselective, 15) regioselective, 16) chemoselective, 18) buffered soln., 21) buffered soln.

RX(465) OF 473 - 23 STEPS



(step 19.2) (step 22.2)

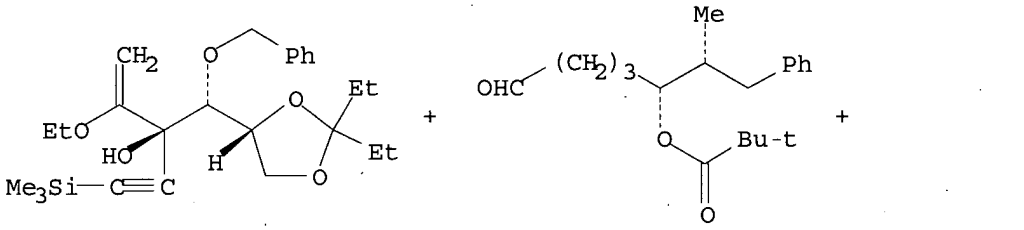
RX(465) OF 473 - 23 STEPS

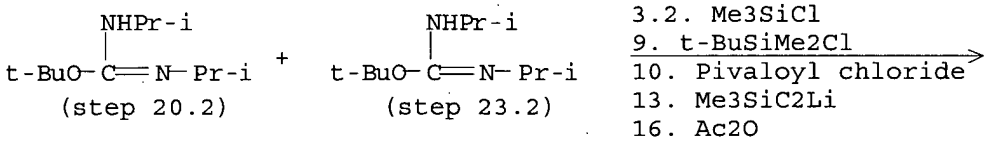


97%

NOTE: 1) chemoselective (stage 1), 2) regioselective, scalable, 5) stereoselective, chemoselective, 7) stereoselective, 8) regioselective, 11) Swern oxidn., in-situ generated reagent, 12) stereoselective, 16) regioselective, 17) chemoselective, 19) buffered soln., 22) buffered soln.

RX(466) OF 473 - 24 STEPS

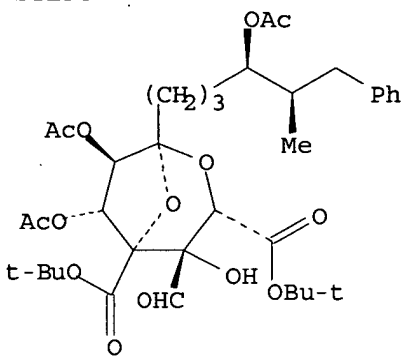




(step 20.2) (step 23.2)

3.1. t-BuSiMe2Cl
3.2. Me3SiCl
9. t-BuSiMe2Cl
10. Pivaloyl chloride
13. Me3SiC2Li
16. Ac2O

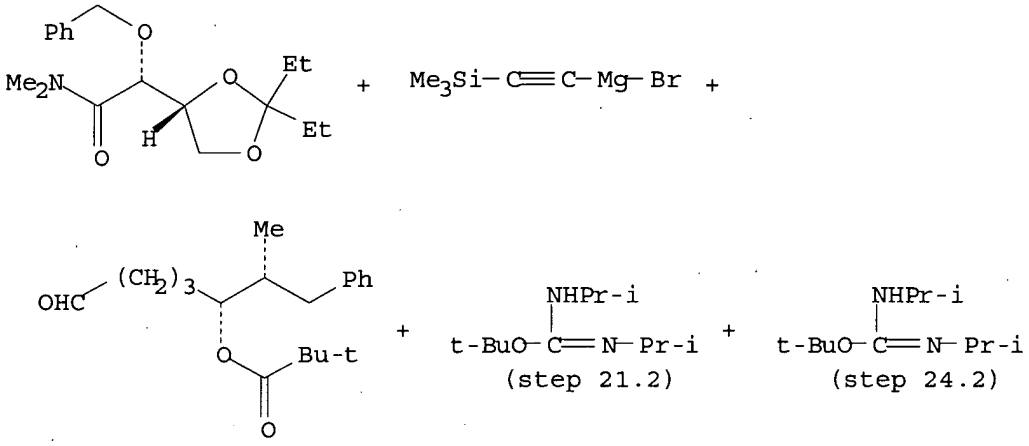
RX(466) OF 473 - 24 STEPS



97%

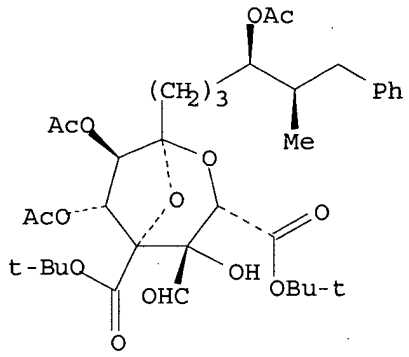
NOTE: 2) chemoselective (stage 1), 3) regioselective, scalable, 6) stereoselective, chemoselective, 8) stereoselective, 9) regioselective, 12) Swern oxidn., in-situ generated reagent, 13) stereoselective, 17) regioselective, 18) chemoselective, 20) buffered soln., 23) buffered soln.

RX(467) OF 473 - 25 STEPS



RX(467) OF 473 - 25 STEPS

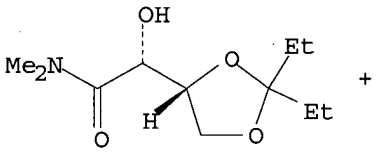
1.1. EtOCH:CH2
4.1. t-BuSiMe2Cl
4.2. Me3SiCl
10. t-BuSiMe2Cl
11. Pivaloyl chloride
14. Me3SiC2Li
17. Ac2O



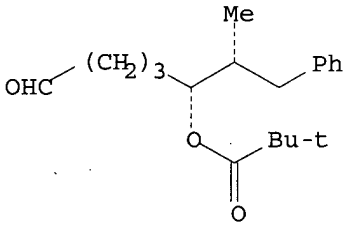
97%

NOTE: 1) stereoselective, 3) chemoselective (stage 1), 4) regioselective, scalable, 7) stereoselective, chemoselective, 9) stereoselective, 10) regioselective, 13) Swern oxidn., in-situ generated reagent, 14) stereoselective, 18) regioselective, 19) chemoselective, 21) buffered soln., 24) buffered soln.

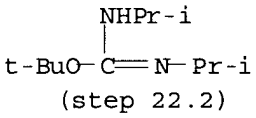
RX(468) OF 473 - 26 STEPS



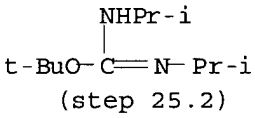
+ $Me_3Si-C\equiv C-Mg-Br$ (step 2.2) +



+



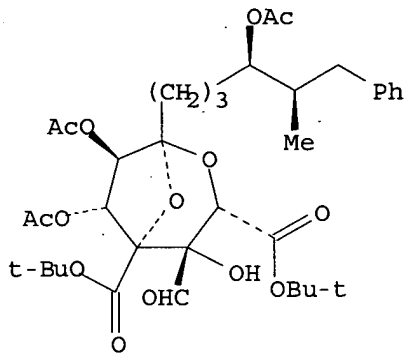
(step 22.2) +



(step 25.2)

RX(468) OF 473 - 26 STEPS

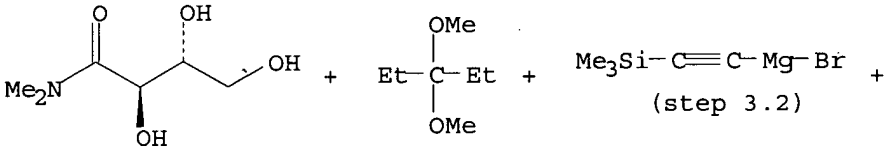
1. PhCH2Cl
2.1. EtOCH:CH2
5.1. t-BuSiMe2Cl
5.2. Me3SiCl
11. t-BuSiMe2Cl
12. Pivaloyl chloride
15. Me3SiC2Li
18. Ac2O

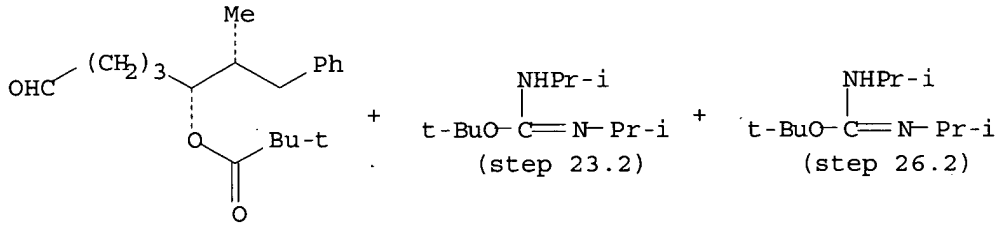


97%

NOTE: 2) stereoselective, 4) chemoselective (stage 1), 5) regioselective, scalable, 8) stereoselective, chemoselective, 10) stereoselective, 11) regioselective, 14) Swern oxidn., in-situ generated reagent, 15) stereoselective, 19) regioselective, 20) chemoselective, 22) buffered soln., 25) buffered soln.

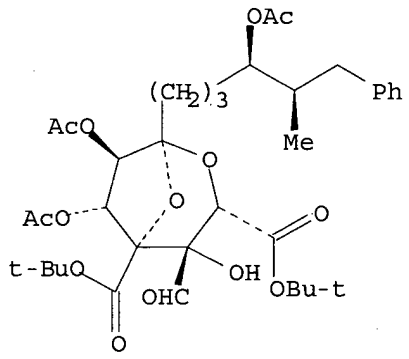
RX(469) OF 473 - 27 STEPS





RX(469) OF 473 - 27 STEPS

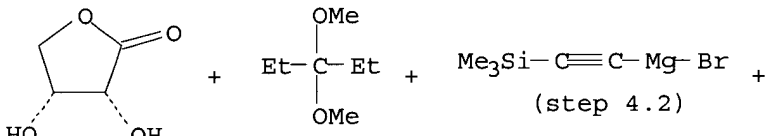
2. PhCH2Cl
3.1. EtOCH:CH2
6.1. t-BuSiMe2Cl
6.2. Me3SiCl
12. t-BuSiMe2Cl
13. Pivaloyl chloride
16. Me3SiC2Li
19. Ac2O

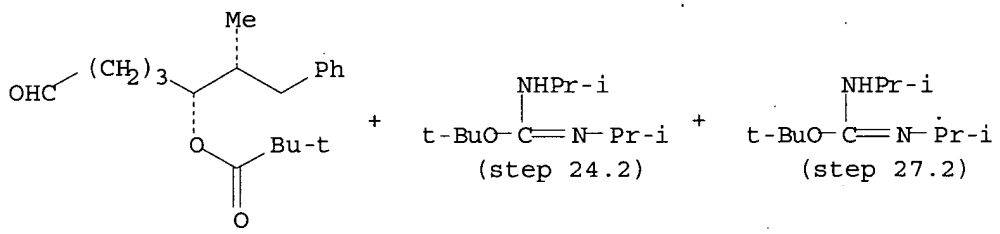


97%

NOTE: 1) regioselective, acidic conditions, 3) stereoselective, 5) chemoselective (stage 1), 6) regioselective, scalable, 9) stereoselective, chemoselective, 11) stereoselective, 12) regioselective, 15) Swern oxidn., in-situ generated reagent, 16) stereoselective, 20) regioselective, 21) chemoselective, 23) buffered soln., 26) buffered soln.

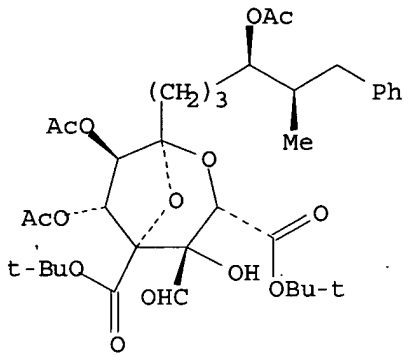
RX(470) OF 473 - 28 STEPS





RX(470) OF 473 - 28 STEPS

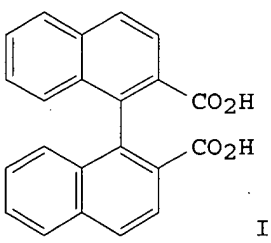
1. Me2NH
3. PhCH2Cl
4.1. EtOCH:CH2
7.1. t-BuSiMe2Cl
7.2. Me3SiCl
13. t-BuSiMe2Cl
14. Pivaloyl chloride
17. Me3SiC2Li
20. Ac2O



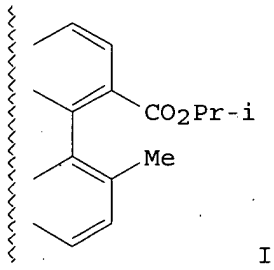
97%

NOTE: 2) regioselective, acidic conditions, 4) stereoselective, 6) chemoselective (stage 1), 7) regioselective, scalable, 10) stereoselective, chemoselective, 12) stereoselective, 13) regioselective, 16) Swern oxidn., in-situ generated reagent, 17) stereoselective, 21) regioselective, 22) chemoselective, 24) buffered soln., 27) buffered soln.

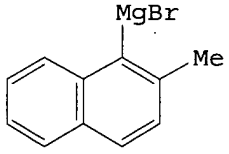
L13 ANSWER 6 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:191277 CASREACT
TITLE: Convenient synthesis of 1,1'-binaphthyl-2,2'-dicarboxylic acid
AUTHOR(S): Oi, Shuichi; Matsunaga, Kenichi; Hattori, Tetsutaro; Miyano, Sotaro
CORPORATE SOURCE: Fac. Eng., Tohoku Univ., Sendai, 980, Japan
SOURCE: Synthesis (1993), (9), 895-8
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



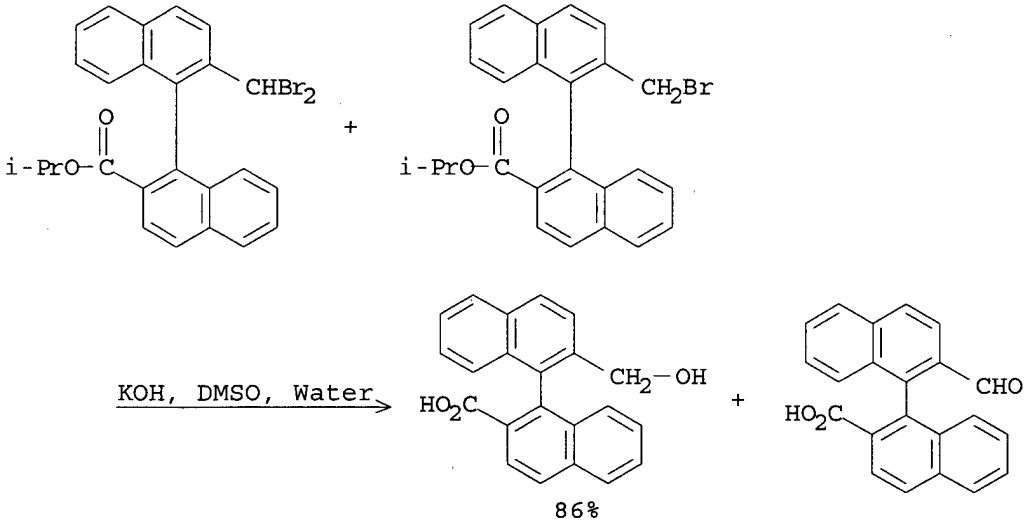
II



III

AB Two syntheses of title compound I in good yields are presented via the oxidation of the 2'-Me substituent binaphthylcarboxylate II, which is readily obtainable by reaction of naphthyl Grignard III with iso-Pr 1-isopropoxy-2-naphthoate.

RX(5) OF 74



L13 ANSWER 7 OF 12 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 116:193986 CASREACT

TITLE: Synthesis of 3-vinylcephalosporins and their 1,3-dipolar cycloaddition reactions with diazo alkanes

AUTHOR(S): Pitlik, Janos; Batta, Gyula; Sztaricskai, Ferenc; Erdodi Kover, Katalin

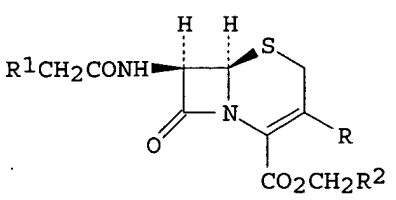
CORPORATE SOURCE: Antibiot. Kem. Kutatocsoport, MTA, Debrecen, 4010, Hung.

SOURCE: Magyar Kemiai Folyoirat (1991), 97(12), 493-509
CODEN: MGKFA3; ISSN: 0025-0155

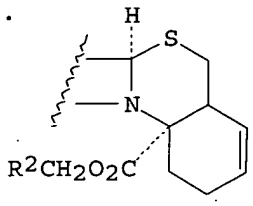
DOCUMENT TYPE: Journal

LANGUAGE: Hungarian

GI



I



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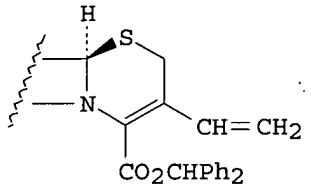
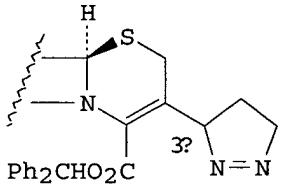
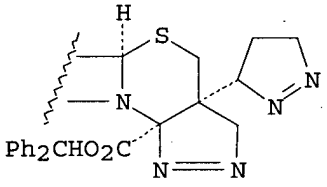


III



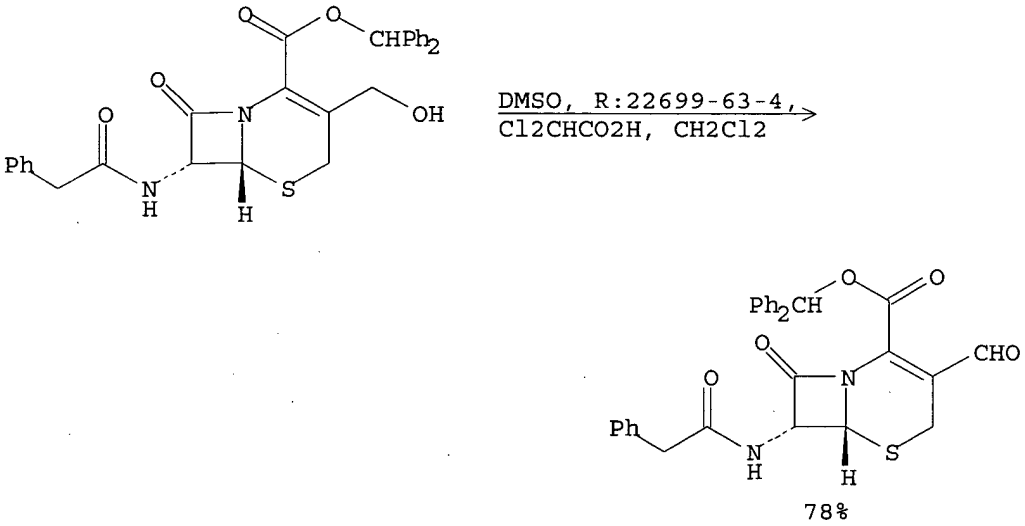
IV



V

AB Chromatog. inseparable mixts. of cis/trans isomers of 3-vinylcephalosporins I (R = e.g., CH:CHR3 with R3 = H, Me, heteroaryl; R1 = Ph, PhO; R2 = H, vinyl) were prepared in up to 81% total yield by iodination of acetoxymethyl derivs. I (R = CH2OAc) with Me3SiI and conversion of the corresponding iodomethyl derivs. to phosponium iodide Wittig reagents for subsequent olefination with R3CHO. Substituent R3 = Me favored the corresponding cis-3-vinylcephalosporin in ratio 5:1, whereas heteroaryl aldehydes resulted in predominantly trans mixts. Wittig reaction with acrolein afforded tricyclic derivative II whose 4-R configuration was established on the basis of mol. modeling calcns. Me3SiI was also applied to the reduction of cephalosporin-1S(β) sulfoxides, affording, e.g., the acetoxymethyl derivs. I (R = CH2OAc, R1 = Ph, PhO; R2 = H) in 65 and 75% yields, resp. An alternative route to 3-vinylcephalosporins involved Wittig reaction of 3-formylcephalosporins I (R = CHO), themselves prepared by DMSO/dicyclohexylcarbodiimide oxidation of the corresponding hydroxymethyl derivs. I (R = CH2OH). Regio- and stereoselective dipolar cycloaddn. reaction of CH2N2 with III (R1 = Ph) afforded the pyrazolyl β-adduct IV with S configuration at C-3' (NOE-mol. modeling determination) together with pyrazolinopyrazolylcephalosporin V. Similar regio- and stereoselectivity was observed for the reaction of III 1S(β) sulfoxide with CH2N2, affording the corresponding IV sulfoxide.

RX(10) OF 16



NOTE: optimization

L13 ANSWER 8 OF 12 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 111:174558 CASREACT

TITLE: Semisynthetic macrolide antibacterials derived from tylosin. Synthesis of 3-O-acetyl-23-O-demycinosyl-4"-O-isovaleryltylosin and related compounds, as well as the 12,13-epoxy derivatives

AUTHOR(S): Fishman, Andrew G.; Mallams, Alan K.; Rossman, Randall R.

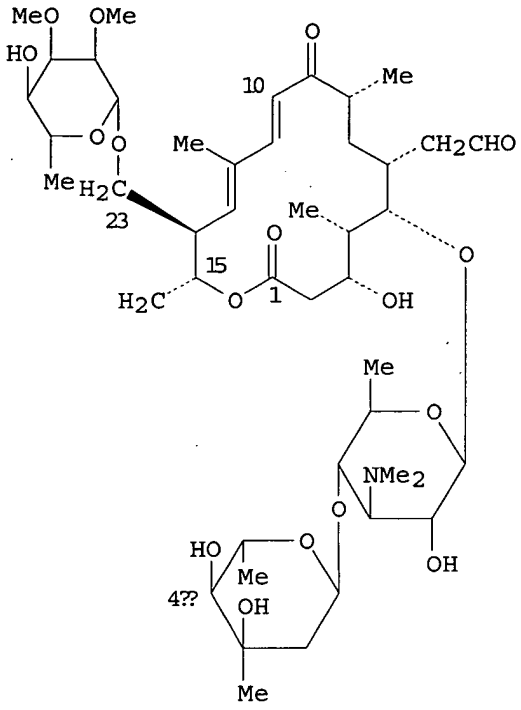
CORPORATE SOURCE: Res. Div., Schering-Plough Corp., Bloomfield, NJ, 07003, USA

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (4), 787-98
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

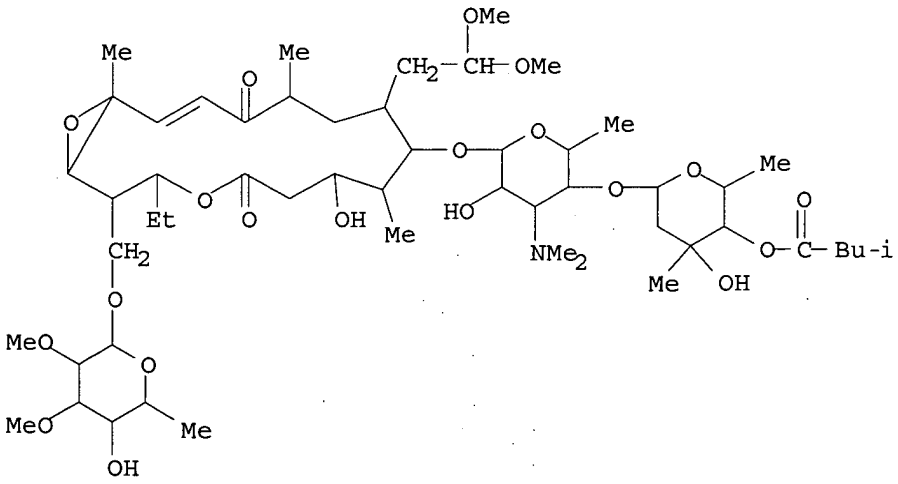
GI



I

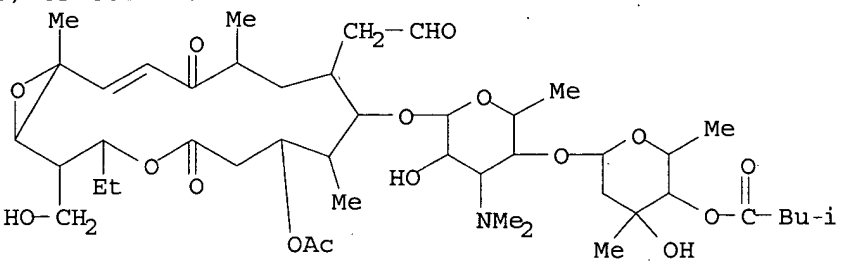
AB Selective acylation techniques have been developed that enable the synthesis of 3-O-acetyl-4''-O-isovaleryltylosin and 3-O-acetyl-23-O-demycinosyl-4''-O-isovaleryltylosin to be carried out in an efficient manner starting from tylosin (I). The 2'--O-acetyl, 23-O-acetyl, and 2',23-di-O-acetyl derivs. of the latter were also prepared, as were key hydrazones. The regio- and stereoselective epoxidn. of tylosin and its acyl derivs. afforded the 12,13-epoxy analogs, which were used to synthesize novel acylated 12,13-epoxy derivs. of 23-O-demycinosyltylosin.

RX(853) OF 862 - 5 STEPS



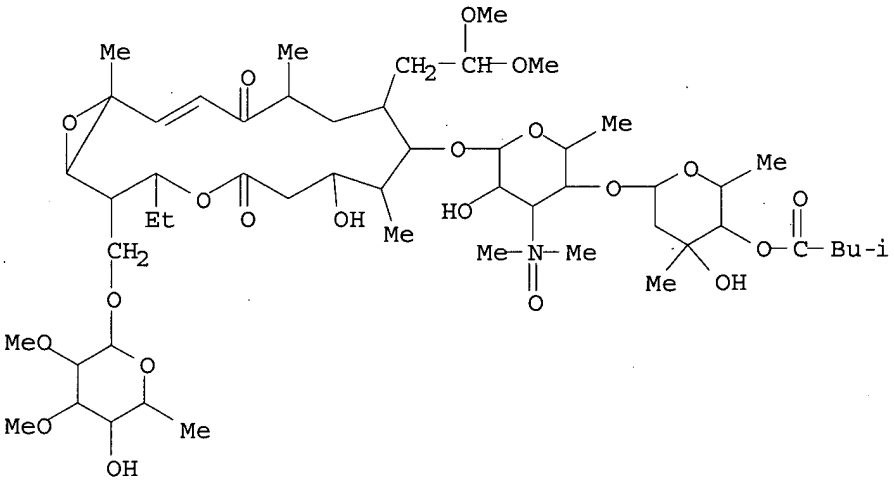
2. Ac2O
4. Ac2O

RX(853) OF 862 - 5 STEPS



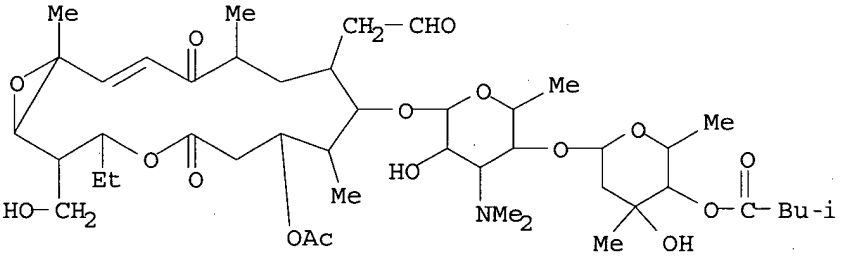
66%

RX(854) OF 862 - 6 STEPS



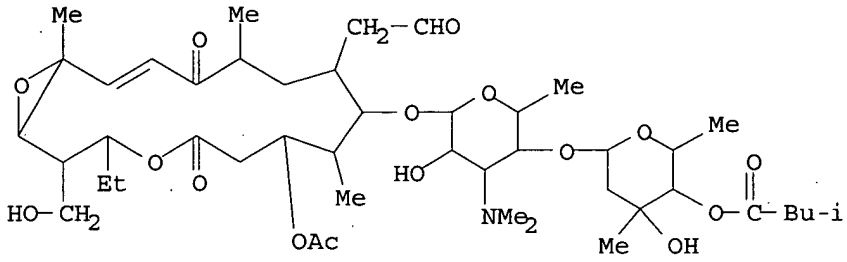
3. Ac2O
5. Ac2O

RX(854) OF 862 - 6 STEPS



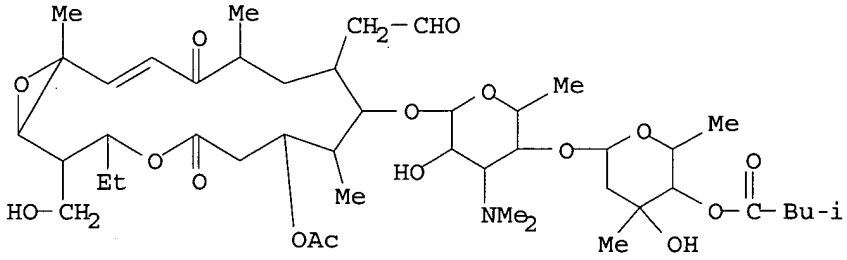
66%

RX(855) OF 862 - 7 STEPS
MULTI
PAGE 4. Ac2O → 6. Ac2O
IMAGE
122076-92-0



66%

RX(856) OF 862 - 8 STEPS
MULTI
PAGE 1. MeOH → 5. Ac2O → 7. Ac2O
IMAGE
63408-91-3



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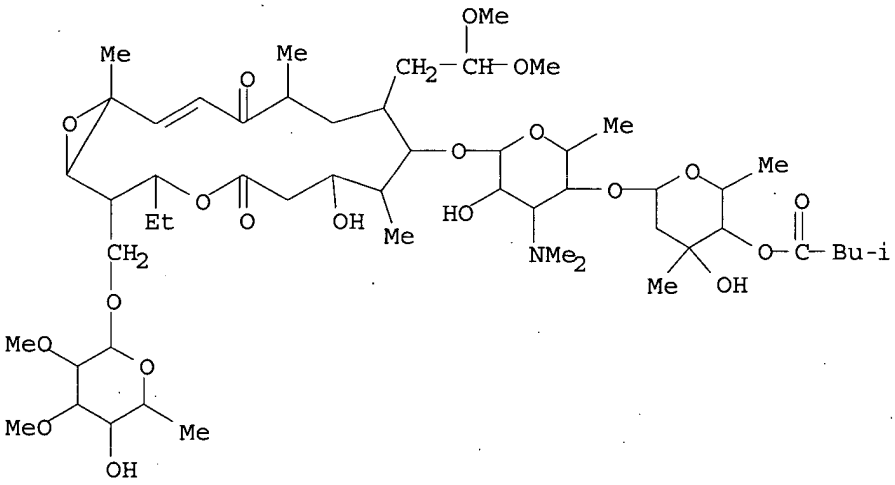
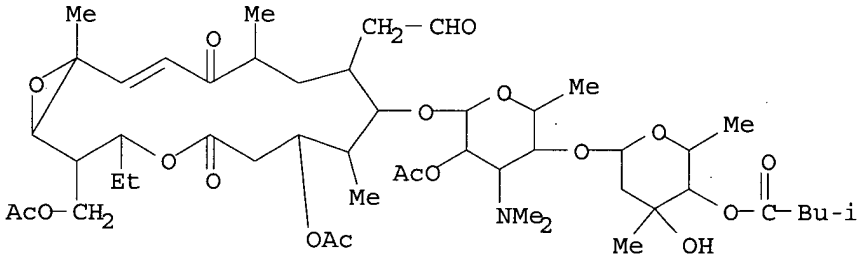
RX(858) OF 862 - 6 STEPS



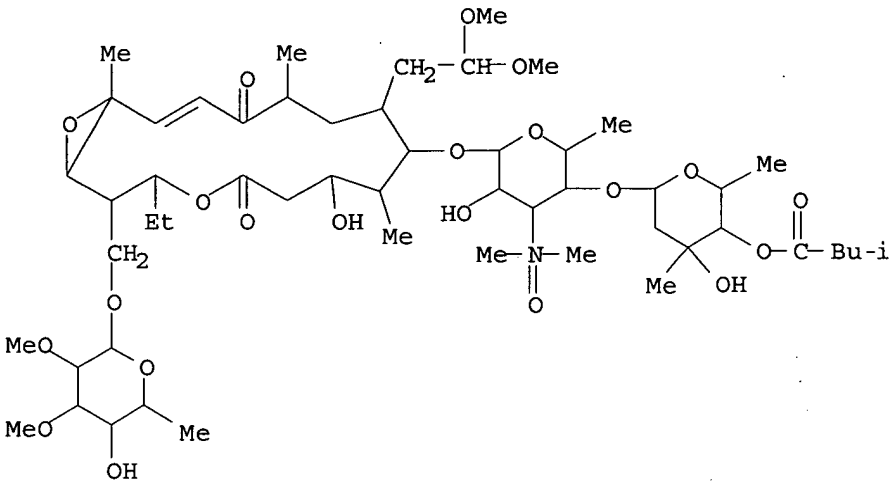
2. Ac2O
4. Ac2O
6. Ac2O

RX(858) OF 862 - 6 STEPS



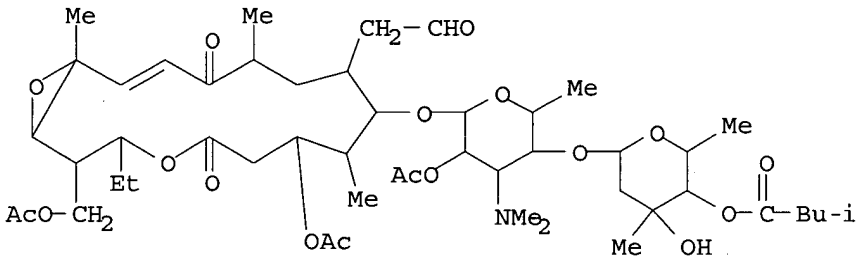
88%

RX(859) OF 862 - 7 STEPS



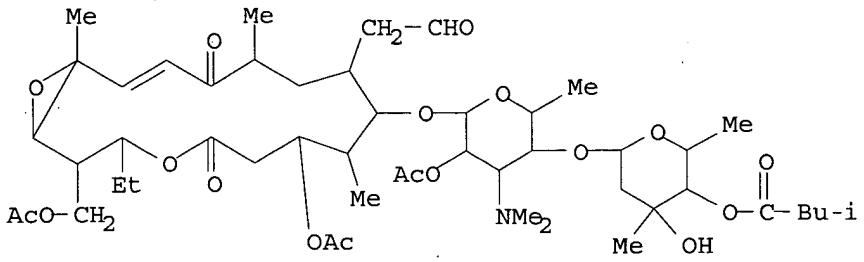
3. Ac2O
5. Ac2O
7. Ac2O

RX(859) OF 862 - 7 STEPS



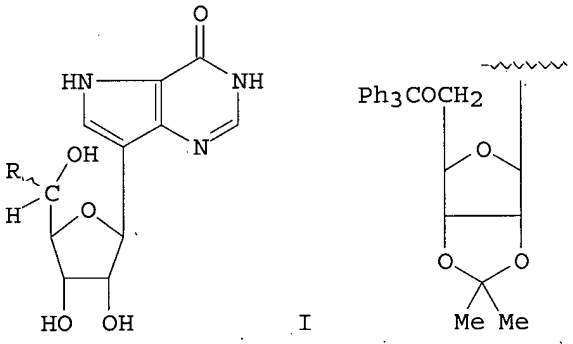
88%

RX(860) OF 862 - 8 STEPS
MULTI
PAGE
IMAGE
4. Ac2O
6. Ac2O
8. Ac2O
122076-92-0



88%

L13 ANSWER 9 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 110:193300 CASREACT
TITLE: Synthesis of tritium-labeled 9-deazainosine
AUTHOR(S): Singh, Ambarish K.; Klein, Robert S.
CORPORATE SOURCE: Lab. Org. Chem., Mem. Sloan-Kettering Cancer Cent., New York, NY, 10021, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(11), 1219-28
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



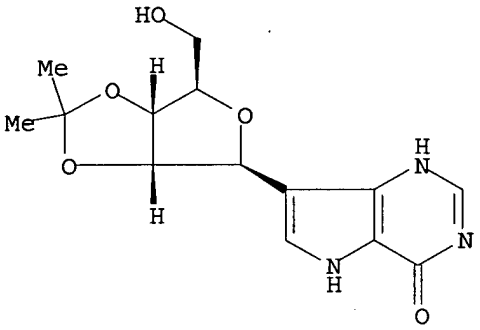
I

II

AB The synthesis of labeled 9-deazainosine I (R = 3H, 2H) from the fully blocked 9-deazainosine II is achieved in six steps by selective detritylation, oxidation of the C-5' hydroxyl group, followed by purification via its N,N'-diphenylimidazolidine derivative, deprotection to obtain the 5'-aldehyde, [3H]-NaBH4 reduction (treatment with NaBD4 to reduce unreacted aldehyde), and deisopropylidenation to give the labeled nucleoside. The sequence is of general utility in labeling nucleosides at the C-5'

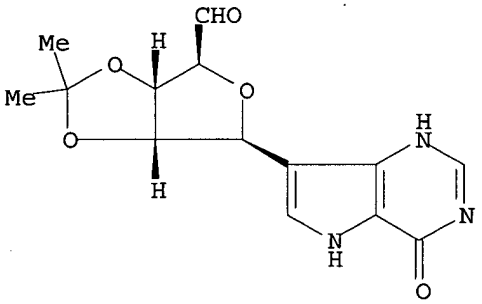
position for biochem. studies.

RX(27) OF 67 - 3 STEPS

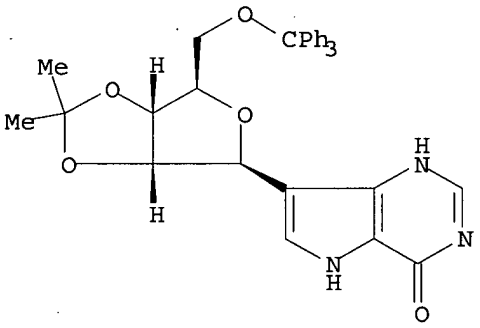


+ PhNH—CH_2—CH_2—NHPh

1.1. DMSO, Cl2CHCO2H, DCC
1.2. MeOH
2. Bio-Rad AG 50W-X8, THF, Water
3. Benzene

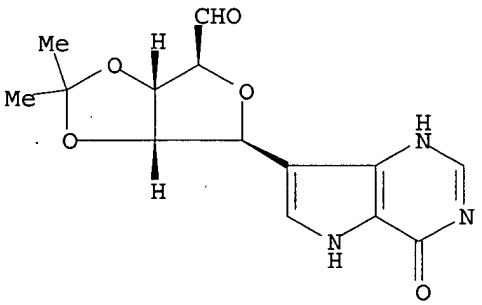


RX(28) OF 67 - 4 STEPS

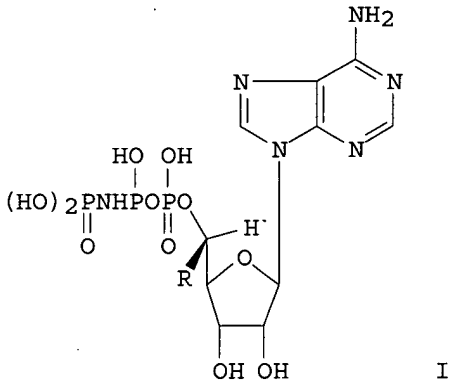


+ PhNH—CH_2—CH_2—NHPh
(step 2.2)

1.1. TsOH, CH2Cl2
1.2. NaHCO3, Water
2.1. DMSO, Cl2CHCO2H, DCC
2.2. MeOH
3. Bio-Rad AG 50W-X8, THF, Water
4. Benzene



L13 ANSWER 10 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 110:173727 CASREACT
TITLE: Approaches to isozyme-specific inhibitors. 16. A novel methyl-C5' covalent adduct of L-ethionine and β,γ-imido-ATP as a potent multisubstrate inhibitor of rat methionine adenosyltransferases
AUTHOR(S): Vrudhula, Vivekananda M.; Kappler, Francis; Afshar, Carol; Ginell, Stephan L.; Lessinger, Leslie; Hampton, Alexander
CORPORATE SOURCE: Fox Chase Cancer Cent., Inst. Cancer Res., Philadelphia, PA, 19111, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(4), 885-90
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

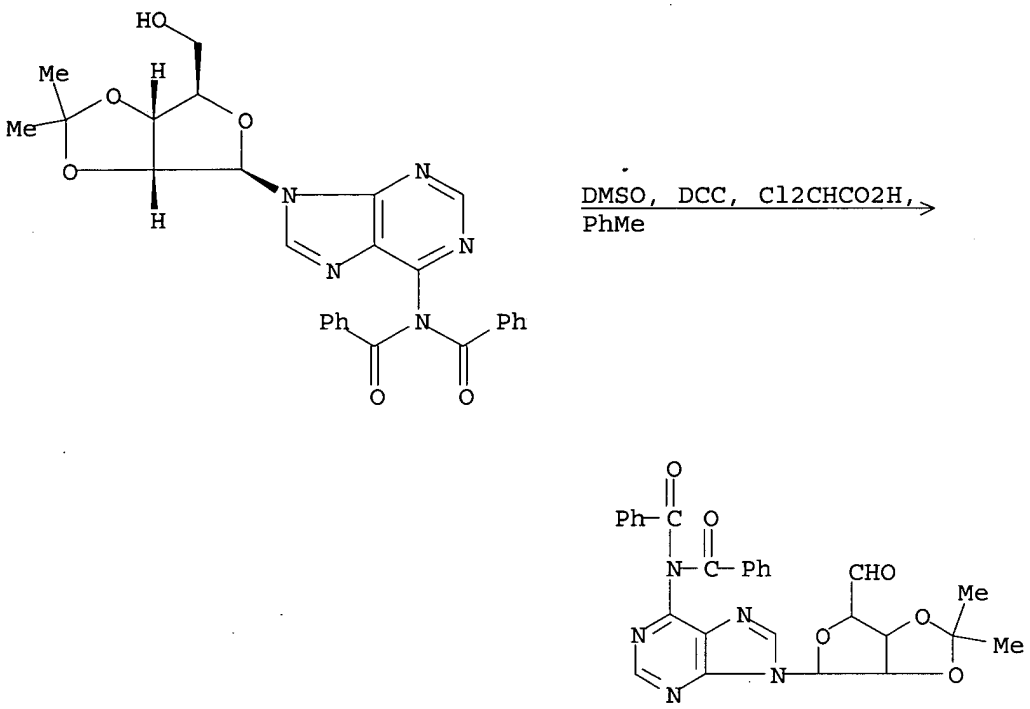


I

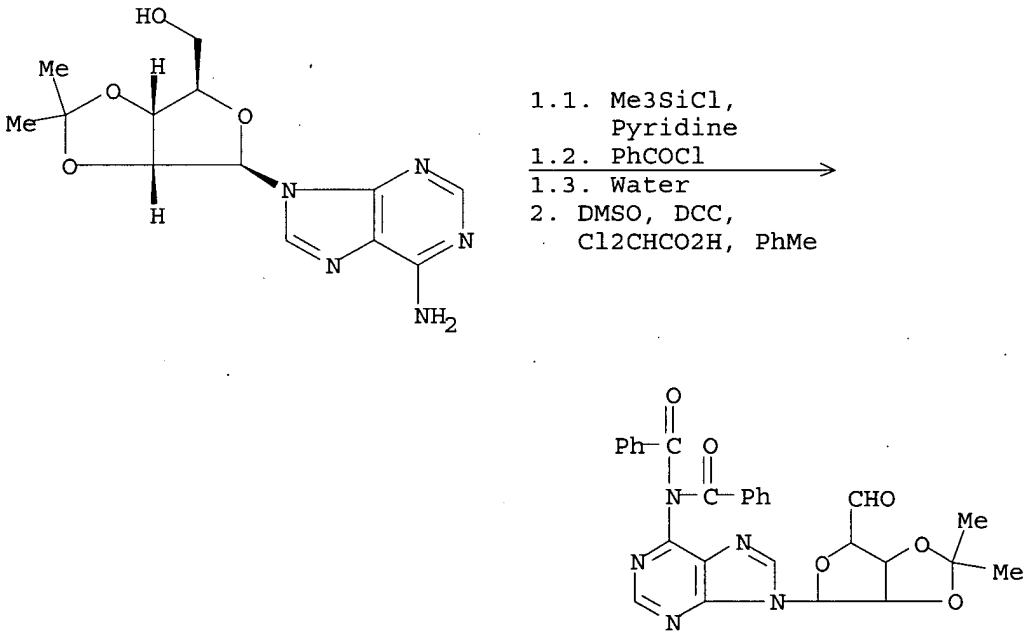
AB N6,N6-Dibenzoyl-2',3'-O-isopropylideneadenosine, which is readily synthesized by one-pot 5'-O-trimethylsilylation, N6-benzoylation, and desilylation, was converted to the corresponding 5'-aldehyde. This was treated with CH2:CHMgBr to afford, after debenzoylation, a 1:3 mixture of the 5'S and 5'R epimers, resp., of 5'-C-vinyl-2',3'-O-isopropylideneadenosine. The configurations were established by single-crystal x-ray diffraction anal. of the 5'R epimer. Hydroboration of the 5'-O-tetrahydropyranyl derivative of the mixed epimeric 5'-C-vinyl nucleosides readily furnished 5'(S,R)-C-(2-hydroxyethyl)-2',3'-O-isopropylideneadenosine. Treatment of the 5'(S,R)-C(2-O-tosyl) derivative of this with disodium L-homocysteinate permitted facile introduction of the L-ethionine system. The α-amino acid group was protected, a β,γ-imidotriphosphoryl group was introduced at O5', and blocking groups were removed to give the title adduct I [R = (CH2)n-(L)-SCH2CH2CH(NH2)CO2H, n = 2] (II), as a 2:3 mixture of its two 5' epimers. II was a powerful inhibitor [KM(ATP)/Ki = 520 and 340] of the M-2 (normal tissue) and M-T (hepatoma tissue) forms, resp., of the title enzyme and displayed predominantly competitive kinetics with the two substrates L-methionine and MgATP. II inhibited M-2 and M-T slightly less effectively than I (n = 1), and gave kinetic evidence of an increased

tendency to form L-methionine-enzyme-adduct and MgATP-enzyme-adduct complexes.

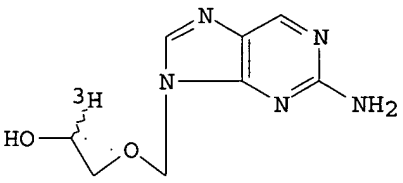
RX(2) OF 47



RX(14) OF 47 - 2 STEPS



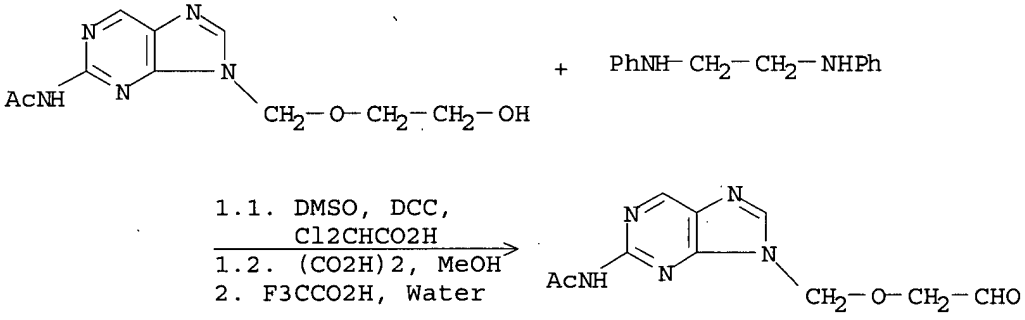
L13 ANSWER 11 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 110:173659 CASREACT
TITLE: Synthesis of [3H]-desciclovir, prodrug of the antiviral acyclovir
AUTHOR(S): Moorman, Allan R.; Hill, John A.
CORPORATE SOURCE: Dep. Exp. Ther., Wellcome Res. Lab., Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(9), 963-9
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

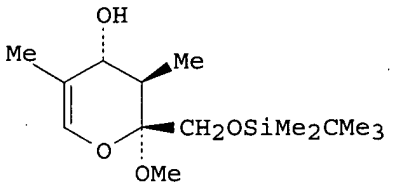
AB The title compound I was prepared by direct radiochem. synthesis from 2-acetylamino-9-[(2-hydroxyethoxy)methyl]-9H-purine. The product had a specific activity of 21.5 Ci mmol-1 and a radiochem. purity of 99.2%.

RX(5) OF 10 - 2 STEPS



L13 ANSWER 12 OF 12 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 102:203790 CASREACT
TITLE: Convergent synthesis of polyether ionophore antibiotics: an approach to the synthesis of the monensin tetrahydropyran-bis(tetrahydrofuran) via the ester enolate Claisen rearrangement and reductive decarboxylation
AUTHOR(S): Ireland, Robert E.; Norbeck, Daniel W.; Mandel, Gretchen S.; Mandel, Neil S.
CORPORATE SOURCE: Chem. Lab., California Inst. Technol., Pasadena, CA,

91125, USA
SOURCE: Journal of the American Chemical Society (1985), 107(11), 3285-94
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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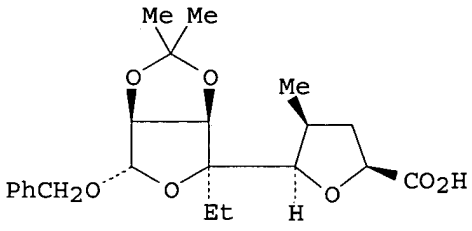
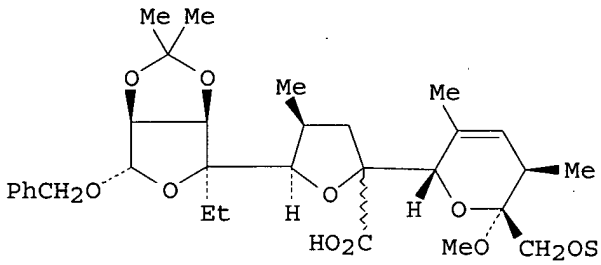


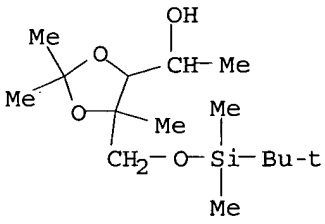
II



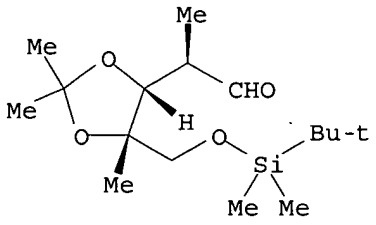
III

AB The monensin tetrahydropyran equivalent I was prepared from D-fructose and then joined to the monensin bis(tetrahydrofuran) equivalent II via the ester enolate Claisen rearrangement. The radical induced, reductive decarboxylation of the resulting acid III was carried out via the phenylseleno ester. Anomeric stabilization of the intermediate tetrahydrofuran-2-yl radical is an important factor in the stereochem. outcome of this process. Reduction of 1-chloro-2,3-O-isopropylidene furanoid and pyranoid carbohydrate derivs. with lithium di-tert-butylbiphenyl affords the corresponding glycals in high yield.

RX(95) OF 631 - 4 STEPS

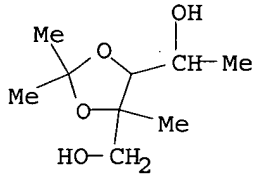


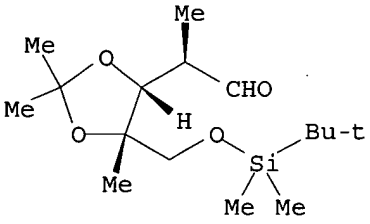
1. Cl2CHCO2H, i-PrN:C:NPr-i, DMSO, Benzene
2. Ph3PMe.Br, BuLi, THF
3.1. BH3, THF
3.2. H2O2, Water
4.1. (COCl)2, DMSO, CH2Cl2
4.2. Et3N



stereoisomers

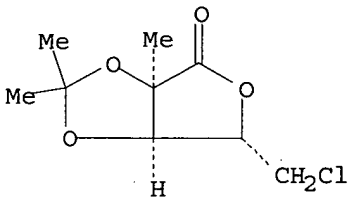
RX(182) OF 631 - 5 STEPS



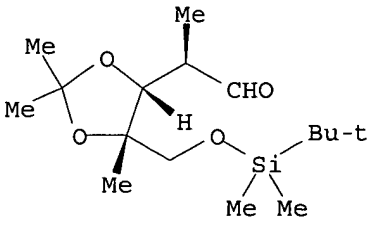


stereoisomers

RX(183) OF 631 - 6 STEPS

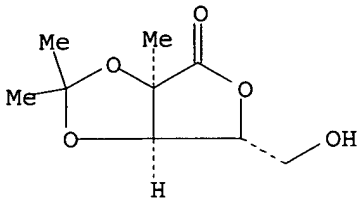


2. t-BuSiMe2Cl
4. Ph3PMe.Br

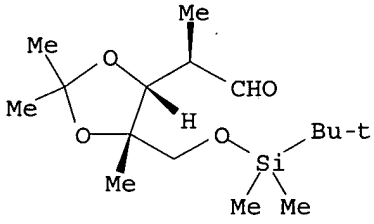


stereoisomers

RX(185) OF 631 - 7 STEPS

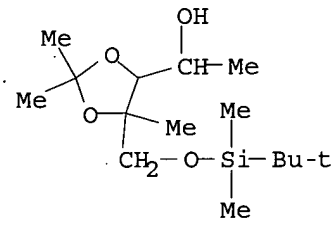


3. t-BuSiMe2Cl
5. Ph3PMe.Br

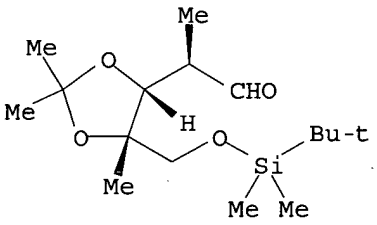


stereoisomers

RX(190) OF 631 - 5 STEPS

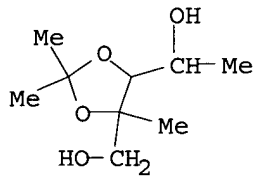


2. Ph3PMe.Br

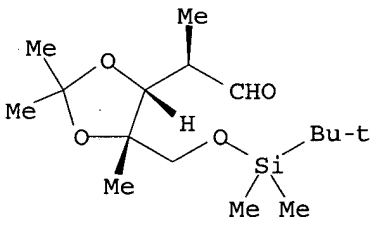


NOTE: 5) silica gel

RX(194) OF 631 - 6 STEPS

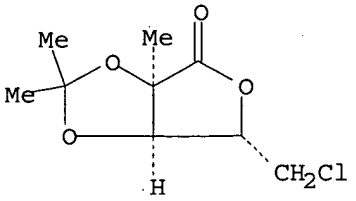


1. t-BuSiMe2Cl
3. Ph3PMe.Br

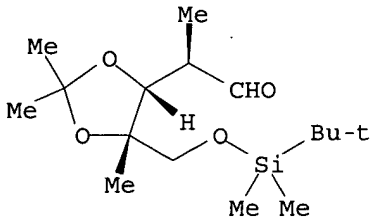


NOTE: 6) silica gel

RX(198) OF 631 - 7 STEPS

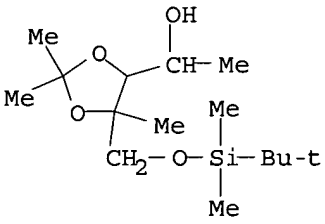


2. t-BuSiMe2Cl
4. Ph3PMe.Br

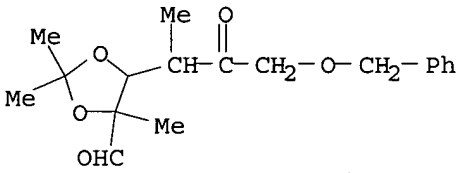


NOTE: 7) silica gel

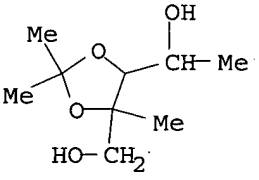
RX(206) OF 631 - 7 STEPS



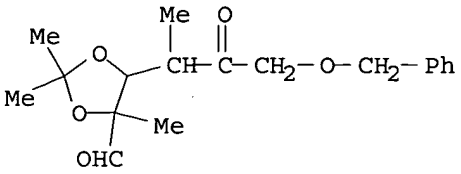
2. Ph3PMe.Br
5. Bu3SnCH2OCH2Ph



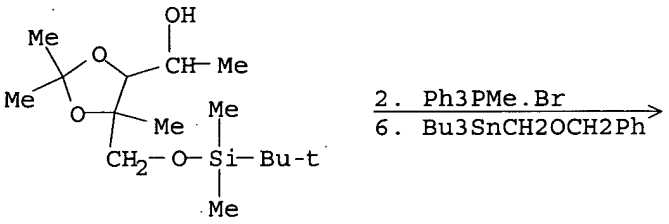
RX(208) OF 631 - 8 STEPS



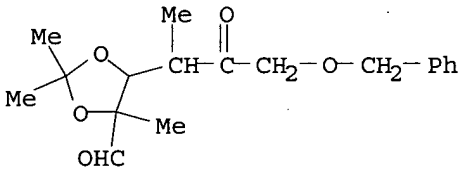
1. t-BuSiMe2Cl
3. Ph3PMe.Br
6. Bu3SnCH2OCH2Ph



RX(220) OF 631 - 8 STEPS

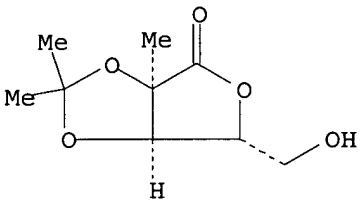


2. Ph3PMe.Br
6. Bu3SnCH2OCH2Ph

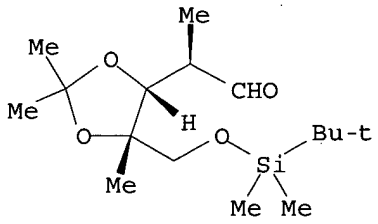


NOTE: 5) silica gel

RX(403) OF 631 - 8 STEPS

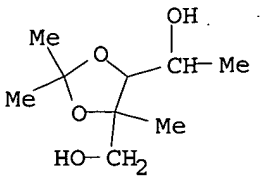


3. t-BuSiMe2Cl
5. Ph3PMe.Br

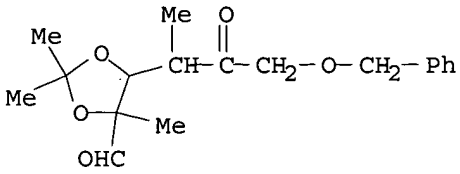


NOTE: 8) silica gel

RX(417) OF 631 - 9 STEPS

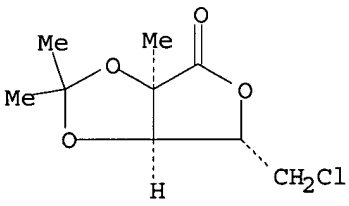


1. t-BuSiMe2Cl
3. Ph3PMe.Br
7. Bu3SnCH2OCH2Ph

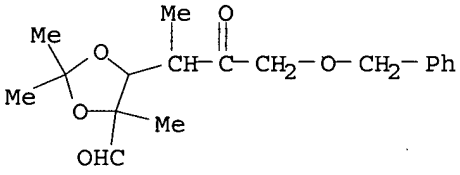


NOTE: 6) silica gel

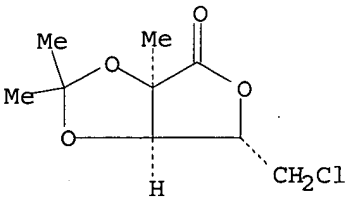
RX(419) OF 631 - 9 STEPS



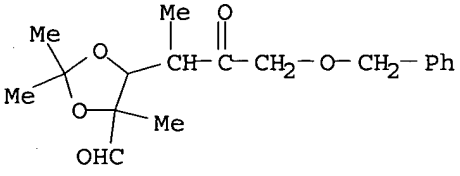
2. t-BuSiMe2Cl
4. Ph3PMe.Br
7. Bu3SnCH2OCH2Ph



RX(421) OF 631 - 10 STEPS

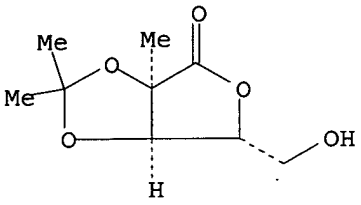


2. t-BuSiMe2Cl
4. Ph3PMe.Br
8. Bu3SnCH2OCH2Ph

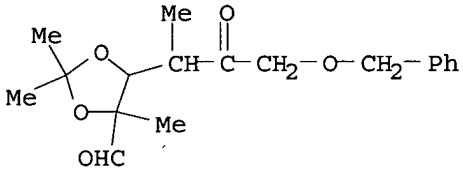


NOTE: 7) silica gel

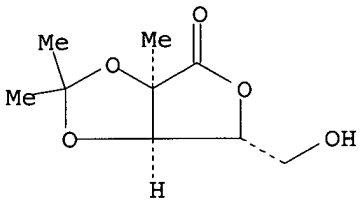
RX(423) OF 631 - 10 STEPS



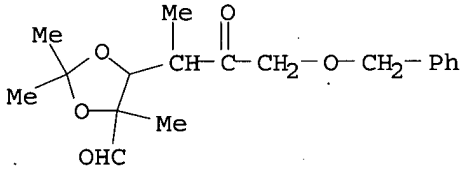
3. t-BuSiMe2Cl
5. Ph3PMe.Br
8. Bu3SnCH2OCH2Ph



RX(425) OF 631 - 11 STEPS



3. t-BuSiMe2Cl
5. Ph3PMe.Br
9. Bu3SnCH2OCH2Ph



NOTE: 8) silica gel

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* available and contains the CA role and document type information.     *
*                                                                       *
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substance identification.

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L19         5539 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SULFOXIDES+PFT,NT/CT(L)(RACT
                 OR RGT OR RCT)/RL
L20          172 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L19
L21              TRANSFER  PLU=ON  L20 1- RN :    4787 TERMS
L22         4787 SEA FILE=REGISTRY ABB=ON  PLU=ON  L21
L23              STR
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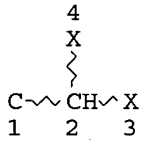


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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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L27            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 AND L20


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L27  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2004:353188  HCAPLUS
DOCUMENT NUMBER:          140:375069
TITLE:                    Process for making an aldehyde by oxidation of
                          dihalomethyl aromatic compound with a sulfoxide
INVENTOR(S):              McKew, John C.; Tam, Steven Y.; Lee, Katherine L.;
                          Chen, Lihren; Thakker, Paresh; Sum, Fuk-Wah; Behnke,
                          Mark; Hu, Baihua; Clark, James D.; Li, Wei
PATENT ASSIGNEE(S):       Wyeth, John, and Brother Ltd., USA
SOURCE:                   U.S. Pat. Appl. Publ., 27 pp., Cont.-in-part of U.S.
                          Pat. Appl. 2003 144,282.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     US 2004082785         A1    20040429    US 2003-722782           20031126
     US 2003144282         A1    20030731    US 2002-302636           20021122
     US 6797708            B2    20040928
PRIORITY APPLN. INFO.:                       US 2001-334588P     P    20011203
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US 2002-302636 A2 20021122

OTHER SOURCE(S): MARPAT 140:375069
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Disclosed is a process for making an aromatic aldehyde of formula AA-CHO (AA = aryl, alkenyl, alkynyl, in particular 2-indolyl of formula Q; R, R3, R4, R9, R10, X2, n3 are defined bellow in formula I) in which a sulfoxide is reacted with a dihalogenated aromatic compound of formula AA-CH(X)X (AA = same as above; X = F, Cl, Br, iodo) in the absence of an effective amount of an activating reagent. The aldehyde may then be used to make other compds., such as a compound [I; R = (CH2)n-A, (CH2)n-S-A, (CH2)n-O-A; A = CH(B)D, CH(B)C; D = C1-6 alkyl or alkoxy, C3-6 cycloalkyl, CF3, (CH2)1-3-CF3; B, C = each (un)substituted Ph, pyridinyl, pyrimidinyl, furanyl, thiophenyl or pyrrolyl; n, n1, n3 = 0-3; X2 = O, CH2, S, SO, SO2, CO, each (un)substituted NH, NHCO, or NHSO2, etc.; R3 = H, halogen, cyano, CHO, CF3, OCF3, OH, C1-6 alkyl, alkoxy, or alkylthio, (un)substituted NH2, NO2, etc.; R4 = H, halogen, cyano, CHO, CF3, OCF3, OH, C1-6 alkyl, alkoxy, or alkylthio, NH2, N(C1-C6 alkyl)2, NH(C1-C6 alkyl), N-C(O)-(C1-C6 alkyl), NO2, N-C(O)-N(C1-C3 alkyl)2, Ph, benzyl, benzyloxy, morpholino, etc. (each ring optionally substituted); R10 = H, C1-6 alkyl; R1 = each (un)substituted C1-6 alkyl, C1-6 fluorinated alkyl, C3-6 cycloalkyl, tetrahydropyranyl, camphoryl, adamantyl, cyano, N(C1-C6 alkyl)2, Ph, pyridinyl, pyrimidinyl, furyl, thienyl, naphthyl, morpholinyl, triazolyl, pyrazolyl, piperidinyl, pyrrolidinyl, imidazolyl, piperidinyl, thiazolidinyl, thiomorpholinyl, tetrazole, indole, benzoxazole, benzofuran, imidazolidine-2-thione, 7,7-dimethylbicyclo[2.2.1]heptan-2-one, benzo[1,2,5]oxadiazole, 2-Oxa-5-azabicyclo[2.2.1]heptane, etc.; X1 = chemical bond, S, O, SO, SO2, NH, NHCO, C:C, etc.; n2 = 0-4] that acts as a cytoplasmic phospholipase A2 (cPLA2) inhibitor. Thus, bromination of 5-chloro-2-methylindole derivative (II; X = Me) by NBS in the presence of benzoyl peroxide in CCl4 under reflux for 3 h gave 2-dibromomethyl-5-chloroindole derivative II (X = CHBr2) which was stirred with DMSO at room temperature for 30 min to quant. give 5-chloro-2-formylindole derivative II (X = CHO).

IC ICM C07D215-38
ICS C07D217-12

INCL 544334000; 546169000; 546146000; 546315000; 548194000; 548236000; 548248000; 568316000

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 7

IT **Aldehydes, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(aromatic; preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

IT **Sulfoxides**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

IT **67-68-5**, DMSO, reactions 75-52-5, Nitromethane, reactions

98-87-3, (Dichloromethyl)benzene **320-65-0**, 1-Dichloromethyl-2-fluorobenzene **402-64-2**, 1-(Dichloromethyl)-3-fluorobenzene **455-34-5**, 1-Dibromomethyl-3-fluorobenzene **618-31-5**, (Dibromomethyl)benzene **6425-24-7**, 1-Dibromomethyl-4-fluorobenzene **26496-95-7**, 4-Dibromomethylbenzoic acid ethyl ester **62037-06-3**, 1-Dibromomethyl-4-chlorobenzene **62247-78-3**, 1-Dibromomethyl-3-bromobenzene **70288-97-0**, 1-Dibromomethyl-3-chlorobenzene **202264-90-2**, 4-Dibromomethylbiphenyl **220141-76-4**, 1-Dibromomethyl-2-fluorobenzene **683812-78-4**, 1-Dibromomethyl-4-ethylbenzene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

IT 4025-75-6P, (4-Nitrophenyl)methanesulfonyl chloride 4352-30-1P, Cyclohexylmethanesulfonyl chloride 24974-73-0P, (3-Chlorophenyl)methanesulfonyl chloride 58032-84-1P, (3-Nitrophenyl)methanesulfonyl chloride 85952-31-4P, (2,6-Dichlorophenyl)methanesulfonyl chloride 92614-55-6P, (2-Methylphenyl)methanesulfonyl chloride 93749-47-4P, 4-(2,2-Diethoxyethoxy)benzoic acid methyl ester 161448-78-8P, (2-Naphthyl)methanesulfonyl chloride 163295-70-3P, (3,5-Dichlorophenyl)methanesulfonyl chloride 163295-71-4P, (2,5-Dichlorophenyl)methanesulfonyl chloride 163295-74-7P, (3,5-Difluorophenyl)methanesulfonyl chloride 163295-76-9P, (3-Methoxyphenyl)methanesulfonyl chloride 174961-63-8P, Methyl 3-[(chlorosulfonyl)methyl]benzoate 179524-60-8P, (2,6-Difluorophenyl)methanesulfonyl chloride 352708-56-6P, (3,5-Dimethylphenyl)methanesulfonyl chloride 479422-23-6P, 4-[2-(5-Chloro-2-methylindol-3-yl)ethoxy]benzoic acid methyl ester 479422-24-7P, 4-[2-(1-Benzhydryl-5-chloro-2-methyl-1H-indol-3-yl)ethoxy]benzoic acid methyl ester 479422-26-9P, 4-[2-(1-Benzhydryl-5-chloro-2-formyl-1H-indol-3-yl)ethoxy]benzoic acid methyl ester 540522-70-1P, 4-[3-[2-(2-Aminoethyl)-1-benzhydryl-5-chloro-1H-indol-3-yl]propyl]benzoic acid methyl ester 540523-00-0P, Methyl 4-[2-[1-benzhydryl-5-chloro-2-[2-[[(2-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoate 540523-96-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(ethenylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 540524-67-2P, (2,6-Dimethylphenyl)methanesulfonyl chloride 683812-85-3P, 4-[2-[1-Benzhydryl-5-chloro-2-(2-nitroethenyl)-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-86-4P, 4-[2-[1-Benzhydryl-2-[2-[(benzylsulfonyl)amino]ethyl]-5-chloro-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-87-5P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(isopropylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-88-6P, 4-[2-[1-Benzhydryl-2-[2-[(butylsulfonyl)amino]ethyl]-5-chloro-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-89-7P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-90-0P, 4-[2-[1-Benzhydryl-2-[2-[[(5-bromo-6-chloro-3-pyridinyl)sulfonyl]amino]ethyl]-5-chloro-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-91-1P 683812-92-2P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[(methylsulfonyl)methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-93-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[2-(1-naphthyl)ethyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-94-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3,4-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-95-5P, 4-[2-[1-Benzhydryl-5-

chloro-2-[2-[[(3,5-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-96-6P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[3-(trifluoromethyl)benzyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-97-7P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[4-(trifluoromethyl)benzyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-98-8P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-fluorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683812-99-9P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-chlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-00-5P, 2-[2-[[(2-Aminobenzyl)sulfonyl]amino]ethyl]-4-[2-(1-benzhydryl-5-chloro-1H-indol-3-yl)ethoxy]benzoic acid methyl ester 683813-01-6P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(dimethylamino)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-02-7P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-naphthylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-03-8P, 3-[[[[2-[1-Benzhydryl-3-[2-(4-methoxycarbonylphenoxy)ethyl]-5-chloro-1H-indol-2-yl]ethyl]amino]sulfonyl]methyl]benzoic acid methyl ester 683813-04-9P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[((E)-2-phenylethenyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-05-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(trifluoromethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-06-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(cyclopropylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-07-2P, 4-[2-[1-Benzhydryl-2-[2-[[[3,5-bis(trifluoromethyl)benzyl]sulfonyl]amino]ethyl]-5-chloro-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-08-3P, 2-[[[2-[1-Benzhydryl-3-[2-(4-methoxycarbonylphenoxy)ethyl]-5-chloro-1H-indol-2-yl]ethyl]amino]sulfonyl]benzoic acid methyl ester 683813-09-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(2-naphthylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-10-7P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3,5-dichlorophenyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-11-8P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3,4-dichlorophenyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-12-9P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2,3-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-13-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2,4-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-14-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-chloro-2-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-15-2P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-cyanobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-16-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3,5-difluorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-17-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3-cyanobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-18-5P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-cyanobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-19-6P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[4-(1-piperidinylsulfonyl)benzyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-20-9P, 4-[2-[2-[2-[[[4-(Aminosulfonyl)benzyl]sulfonyl]amino]ethyl]-1-benzhydryl-5-chloro-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-21-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[4-(methanesulfonyl)phenyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-22-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[4-(diethylsulfamoyl)phenyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-23-2P, 4-[3-(5-Chloro-2-methyl-1H-indol-3-yl)propyl]benzoic acid methyl ester 683813-24-3P, 4-[3-(1-Benzhydryl-5-chloro-2-methyl-1H-indol-

3-yl)propyl]benzoic acid methyl ester 683813-25-4P, 4-[3-(1-Benzhydryl-5-chloro-2-formyl-1H-indol-3-yl)propyl]benzoic acid methyl ester 683813-26-5P, 4-[3-[1-Benzhydryl-5-chloro-2-(2-nitroethenyl)-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-27-6P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(phenylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-28-7P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3,5-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-29-8P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3,4-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-30-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(methylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-31-2P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[(phenylsulfonyl)amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-32-3P, 2-[[[2-[[[2-[1-Benzhydryl-3-[2-(4-methoxycarbonylphenoxy)ethyl]-5-chloro-1H-indol-2-yl]ethyl]amino]sulfonyl]ethyl]amino]carbonyl]benzoic acid methyl ester 683813-33-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-34-5P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-35-6P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-36-7P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(2,6-dimethylbenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-37-8P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(cyclohexylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-38-9P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-39-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-40-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-41-4P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(4-fluorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-42-5P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[[4-(trifluoromethyl)benzyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-43-6P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[[3-(trifluoromethyl)benzyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-44-7P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(4-chlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-45-8P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(2-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-46-9P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-47-0P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(4-pyridinylmethyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-48-1P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(2-chlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-49-2P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-50-5P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3-chlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-51-6P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(2,5-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-52-7P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(3-methoxybenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-53-8P, 4-[3-[2-[2-[[(2-Aminobenzyl)sulfonyl]amino]ethyl]-1-benzhydryl-5-chloro-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-54-9P, 4-[3-[1-Benzhydryl-5-chloro-2-[2-[[(2-

methylbenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]propyl]benzoic acid methyl ester 683813-55-0P, [4-(Trifluoromethoxy)phenyl]methanesulfonyl chloride 683813-56-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(4-trifluoromethoxybenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-57-2P, (4-Fluoro-6-nitrophenyl)methanesulfonyl chloride 683813-58-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-fluoro-6-nitrobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-59-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2,6-difluorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-60-7P, (6-Chloro-3-pyridyl)methanesulfonyl chloride 683813-61-8P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[(6-chloro-3-pyridinyl)methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-62-9P, (5,6-Dichloro-3-pyridyl)methanesulfonyl chloride 683813-63-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[(5,6-dichloro-3-pyridinyl)methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-64-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3-methoxybenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-65-2P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(3,5-dimethylbenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-66-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2-methylbenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-67-4P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[(2,6-dichlorobenzyl)sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-68-5P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[(phenylsulfanyl)methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-69-6P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[(2,6-dimethylphenyl)sulfanyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-70-9P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[(2-methoxyphenyl)sulfanyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-71-0P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[(2-chloro-6-methylphenyl)sulfanyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-72-1P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[(3,5-dichlorophenyl)sulfanyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-73-2P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[[(3,4-dimethoxyphenyl)sulfanyl]methyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester 683813-74-3P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[2-(pyrazol-1-yl)ethyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester **683813-75-4P**, 4-[2-(1-Benzhydryl-5-chloro-2-(dibromomethyl)-1H-indol-3-yl)ethoxy]benzoic acid methyl ester 683813-76-5P, 4-[2-[1-Benzhydryl-5-chloro-2-[2-[[[2-(morpholin-4-yl)ethyl]sulfonyl]amino]ethyl]-1H-indol-3-yl]ethoxy]benzoic acid methyl ester

RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

IT **100-52-7P**, Benzaldehyde, preparation **104-88-1P**, 4-Chlorobenzaldehyde, preparation **446-52-6P**, 2-Fluorobenzaldehyde **456-48-4P**, 3-Fluorobenzaldehyde **459-57-4P**, 4-Fluorobenzaldehyde **587-04-2P**, 3-Chlorobenzaldehyde **3132-99-8P**, 3-Bromobenzaldehyde **3218-36-8P**, 4-Biphenylcarboxaldehyde 4748-78-1P, 4-Ethylbenzaldehyde 6287-86-1P, 4-Formylbenzoic acid ethyl ester

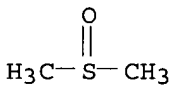
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(preparation of aromatic aldehydes by oxidation of α,α-

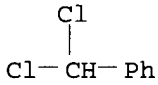
dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

IT **67-68-5**, DMSO, reactions **98-87-3**, (Dichloromethyl)benzene **320-65-0**, 1-Dichloromethyl-2-fluorobenzene **402-64-2**, 1-(Dichloromethyl)-3-fluorobenzene **455-34-5**, 1-Dibromomethyl-3-fluorobenzene **618-31-5**, (Dibromomethyl)benzene **6425-24-7**, 1-Dibromomethyl-4-fluorobenzene **26496-95-7**, 4-Dibromomethylbenzoic acid ethyl ester **62037-06-3**, 1-Dibromomethyl-4-chlorobenzene **62247-78-3**, 1-Dibromomethyl-3-bromobenzene **70288-97-0**, 1-Dibromomethyl-3-chlorobenzene **202264-90-2**, 4-Dibromomethylbiphenyl **220141-76-4**, 1-Dibromomethyl-2-fluorobenzene **683812-78-4**, 1-Dibromomethyl-4-ethylbenzene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)

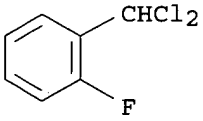
RN 67-68-5 HCAPLUS
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)



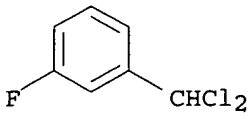
RN 98-87-3 HCAPLUS
CN Benzene, (dichloromethyl)- (9CI) (CA INDEX NAME)



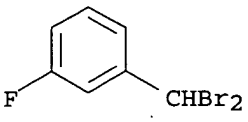
RN 320-65-0 HCAPLUS
CN Benzene, 1-(dichloromethyl)-2-fluoro- (9CI) (CA INDEX NAME)



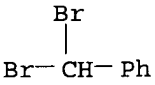
RN 402-64-2 HCAPLUS
CN Benzene, 1-(dichloromethyl)-3-fluoro- (9CI) (CA INDEX NAME)



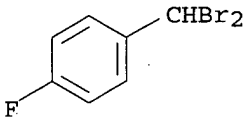
RN 455-34-5 HCAPLUS
CN Benzene, 1-(dibromomethyl)-3-fluoro- (9CI) (CA INDEX NAME)



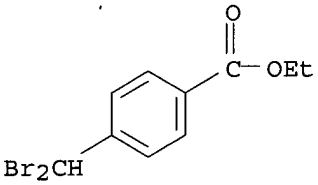
RN 618-31-5 HCAPLUS
CN Benzene, (dibromomethyl)- (9CI) (CA INDEX NAME)



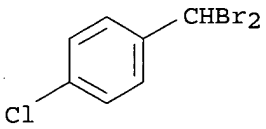
RN 6425-24-7 HCAPLUS
CN Benzene, 1-(dibromomethyl)-4-fluoro- (9CI) (CA INDEX NAME)



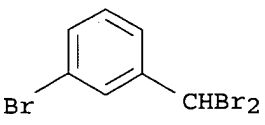
RN 26496-95-7 HCAPLUS
CN Benzoic acid, 4-(dibromomethyl)-, ethyl ester (9CI) (CA INDEX NAME)



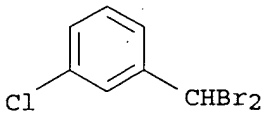
RN 62037-06-3 HCAPLUS
CN Benzene, 1-chloro-4-(dibromomethyl)- (9CI) (CA INDEX NAME)



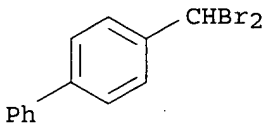
RN 62247-78-3 HCAPLUS
CN Benzene, 1-bromo-3-(dibromomethyl)- (9CI) (CA INDEX NAME)



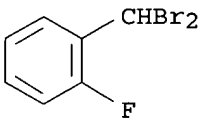
RN 70288-97-0 HCAPLUS
CN Benzene, 1-chloro-3-(dibromomethyl)- (9CI) (CA INDEX NAME)



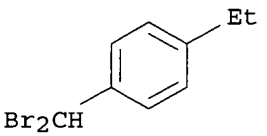
RN 202264-90-2 HCAPLUS
CN 1,1'-Biphenyl, 4-(dibromomethyl)- (9CI) (CA INDEX NAME)



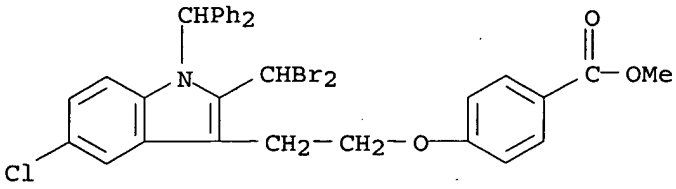
RN 220141-76-4 HCAPLUS
CN Benzene, 1-(dibromomethyl)-2-fluoro- (9CI) (CA INDEX NAME)



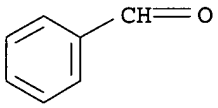
RN 683812-78-4 HCAPLUS
CN Benzene, 1-(dibromomethyl)-4-ethyl- (9CI) (CA INDEX NAME)



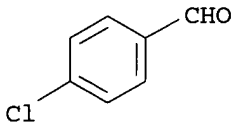
IT **683813-75-4P**, 4-[2-(1-Benzhydryl-5-chloro-2-(dibromomethyl)-1H-indol-3-yl)ethoxy]benzoic acid methyl ester
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)
RN 683813-75-4 HCAPLUS
CN Benzoic acid, 4-[2-[5-chloro-2-(dibromomethyl)-1-(diphenylmethyl)-1H-indol-3-yl]ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



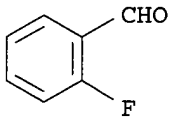
IT **100-52-7P**, Benzaldehyde, preparation **104-88-1P**, 4-Chlorobenzaldehyde, preparation **446-52-6P**, 2-Fluorobenzaldehyde **456-48-4P**, 3-Fluorobenzaldehyde **459-57-4P**, 4-Fluorobenzaldehyde **587-04-2P**, 3-Chlorobenzaldehyde **3132-99-8P**, 3-Bromobenzaldehyde **3218-36-8P**, 4-Biphenylcarboxaldehyde
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of aromatic aldehydes by oxidation of α,α-dihaloarylmethanes with sulfoxides and conversion of indolecarboxaldehydes into N-(indolylmethyl)alkanesulfoxamides useful as cytoplasmic phospholipase A2 inhibitors)
RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



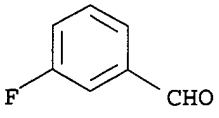
RN 104-88-1 HCAPLUS
CN Benzaldehyde, 4-chloro- (9CI) (CA INDEX NAME)



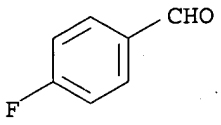
RN 446-52-6 HCAPLUS
CN Benzaldehyde, 2-fluoro- (9CI) (CA INDEX NAME)



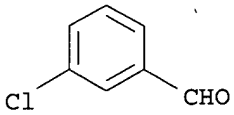
RN 456-48-4 HCAPLUS
CN Benzaldehyde, 3-fluoro- (9CI) (CA INDEX NAME)



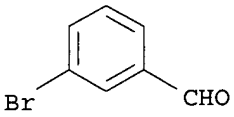
RN 459-57-4 HCAPLUS
CN Benzaldehyde, 4-fluoro- (9CI) (CA INDEX NAME)



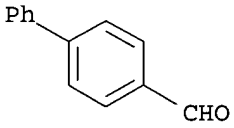
RN 587-04-2 HCAPLUS
CN Benzaldehyde, 3-chloro- (9CI) (CA INDEX NAME)



RN 3132-99-8 HCAPLUS
CN Benzaldehyde, 3-bromo- (9CI) (CA INDEX NAME)

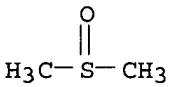


RN 3218-36-8 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxaldehyde (9CI) (CA INDEX NAME)

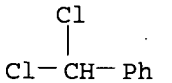


L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:40052 HCAPLUS
DOCUMENT NUMBER: 140:423430
TITLE: Oxygen transfer from sulfoxide. Formation of aromatic aldehydes from dihalomethylarenes
AUTHOR(S): Li, Wei; Li, Jianchang; DeVincentis, Dianne; Mansour, Tarek S.
CORPORATE SOURCE: Chemical and Screening Sciences, Wyeth Research, Cambridge, MA, 02140, USA
SOURCE: Tetrahedron Letters (2004), 45(5), 1071-1074
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The conversion of dihalomethylarenes to the corresponding aldehydes is accomplished conveniently by using sulfoxides as the oxygen donor under neutral conditions.

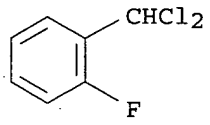
CC 25-15 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Aldehydes, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(aromatic; preparation of aromatic aldehydes from dihalomethylarenes by oxygen
transfer from sulfoxide)
IT **67-68-5**, DMSO, reactions **98-87-3**, Benzal chloride
320-65-0, o-Fluorobenzal chloride **402-64-2**,
m-Fluorobenzal chloride **455-34-5**, 3-Fluorobenzal bromide
535-15-9, Ethyl dichloroacetate **618-31-5**, Benzal bromide
2648-61-5, 2,2-Dichloroacetophenone **6425-24-7**
26496-95-7, Ethyl 4-dibromomethylbenzoate **30263-65-1**
62037-06-3, 4-Chlorobenzal bromide **62247-78-3**,
3-Bromobenzal bromide **70288-97-0**, 3-Chlorobenzal bromide
202264-90-2 220141-76-4
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes from dihalomethylarenes by oxygen transfer
from sulfoxide)
IT **100-52-7P**, Benzaldehyde, preparation **104-88-1P**,
p-Chlorobenzaldehyde, preparation **446-52-6P**,
o-Fluorobenzaldehyde **456-48-4P**, m-Fluorobenzaldehyde
459-57-4P, p-Fluorobenzaldehyde **587-04-2P**,
3-Chlorobenzaldehyde **924-44-7P 1074-12-0P**
3132-99-8P, m-Bromobenzaldehyde **3218-36-8P**,
p-Biphenylaldehyde 4480-47-1P 6287-86-1P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of aromatic aldehydes from dihalomethylarenes by oxygen transfer
from sulfoxide)
IT **67-68-5**, DMSO, reactions **98-87-3**, Benzal chloride
320-65-0, o-Fluorobenzal chloride **402-64-2**,
m-Fluorobenzal chloride **455-34-5**, 3-Fluorobenzal bromide
535-15-9, Ethyl dichloroacetate **618-31-5**, Benzal bromide
2648-61-5, 2,2-Dichloroacetophenone **6425-24-7**
26496-95-7, Ethyl 4-dibromomethylbenzoate **30263-65-1**
62037-06-3, 4-Chlorobenzal bromide **62247-78-3**,
3-Bromobenzal bromide **70288-97-0**, 3-Chlorobenzal bromide
202264-90-2 220141-76-4
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of aromatic aldehydes from dihalomethylarenes by oxygen transfer
from sulfoxide)
RN 67-68-5 HCAPLUS
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)



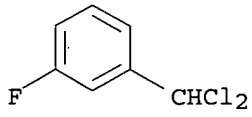
RN 98-87-3 HCAPLUS
CN Benzene, (dichloromethyl)- (9CI) (CA INDEX NAME)



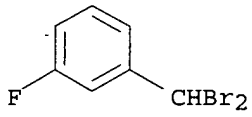
RN 320-65-0 HCAPLUS
CN Benzene, 1-(dichloromethyl)-2-fluoro- (9CI) (CA INDEX NAME)



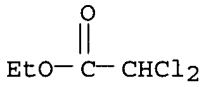
RN 402-64-2 HCAPLUS
CN Benzene, 1-(dichloromethyl)-3-fluoro- (9CI) (CA INDEX NAME)



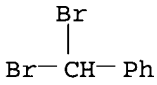
RN 455-34-5 HCAPLUS
CN Benzene, 1-(dibromomethyl)-3-fluoro- (9CI) (CA INDEX NAME)



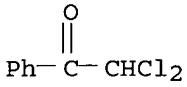
RN 535-15-9 HCAPLUS
CN Acetic acid, dichloro-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



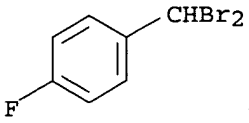
RN 618-31-5 HCAPLUS
CN Benzene, (dibromomethyl)- (9CI) (CA INDEX NAME)



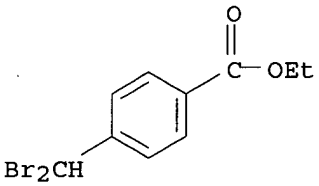
RN 2648-61-5 HCAPLUS
CN Ethanone, 2,2-dichloro-1-phenyl- (9CI) (CA INDEX NAME)



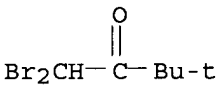
RN 6425-24-7 HCAPLUS
CN Benzene, 1-(dibromomethyl)-4-fluoro- (9CI) (CA INDEX NAME)



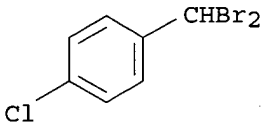
RN 26496-95-7 HCAPLUS
CN Benzoic acid, 4-(dibromomethyl)-, ethyl ester (9CI) (CA INDEX NAME)



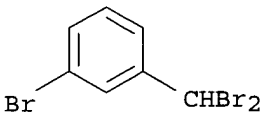
RN 30263-65-1 HCAPLUS
CN 2-Butanone, 1,1-dibromo-3,3-dimethyl- (8CI, 9CI) (CA INDEX NAME)



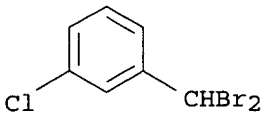
RN 62037-06-3 HCAPLUS
CN Benzene, 1-chloro-4-(dibromomethyl)- (9CI) (CA INDEX NAME)



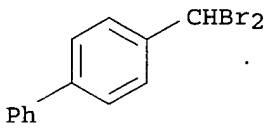
RN 62247-78-3 HCAPLUS
CN Benzene, 1-bromo-3-(dibromomethyl)- (9CI) (CA INDEX NAME)



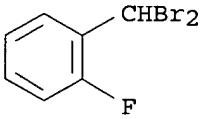
RN 70288-97-0 HCAPLUS
CN Benzene, 1-chloro-3-(dibromomethyl)- (9CI) (CA INDEX NAME)



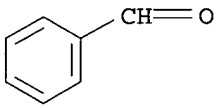
RN 202264-90-2 HCAPLUS
CN 1,1'-Biphenyl, 4-(dibromomethyl)- (9CI) (CA INDEX NAME)



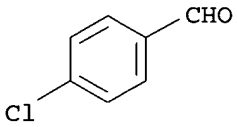
RN 220141-76-4 HCAPLUS
CN Benzene, 1-(dibromomethyl)-2-fluoro- (9CI) (CA INDEX NAME)



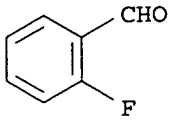
IT **100-52-7P**, Benzaldehyde, preparation **104-88-1P**, p-Chlorobenzaldehyde, preparation **446-52-6P**, o-Fluorobenzaldehyde **456-48-4P**, m-Fluorobenzaldehyde **459-57-4P**, p-Fluorobenzaldehyde **587-04-2P**, 3-Chlorobenzaldehyde **924-44-7P 1074-12-0P** **3132-99-8P**, m-Bromobenzaldehyde **3218-36-8P**, p-Biphenylaldehyde
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of aromatic aldehydes from dihalomethylarenes by oxygen transfer
from sulfoxide)
RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



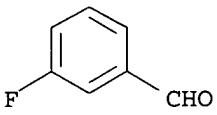
RN 104-88-1 HCAPLUS
CN Benzaldehyde, 4-chloro- (9CI) (CA INDEX NAME)



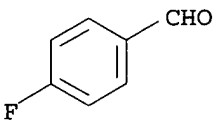
RN 446-52-6 HCAPLUS
CN Benzaldehyde, 2-fluoro- (9CI) (CA INDEX NAME)



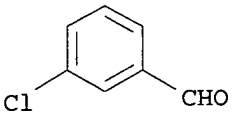
RN 456-48-4 HCAPLUS
CN Benzaldehyde, 3-fluoro- (9CI) (CA INDEX NAME)



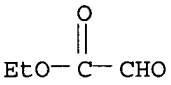
RN 459-57-4 HCAPLUS
CN Benzaldehyde, 4-fluoro- (9CI) (CA INDEX NAME)



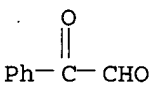
RN 587-04-2 HCAPLUS
CN Benzaldehyde, 3-chloro- (9CI) (CA INDEX NAME)



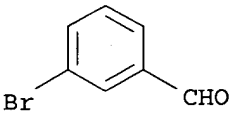
RN 924-44-7 HCAPLUS
CN Acetic acid, oxo-, ethyl ester (9CI) (CA INDEX NAME)



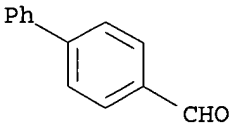
RN 1074-12-0 HCAPLUS
CN Benzeneacetaldehyde, α-oxo- (9CI) (CA INDEX NAME)



RN 3132-99-8 HCAPLUS
CN Benzaldehyde, 3-bromo- (9CI) (CA INDEX NAME)

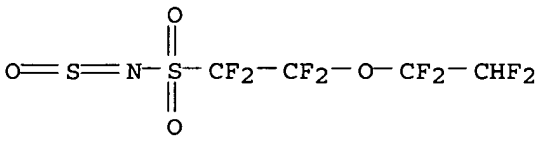


RN 3218-36-8 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxaldehyde (9CI) (CA INDEX NAME)

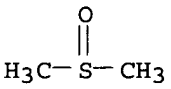


REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

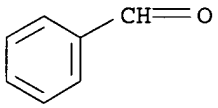
L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:513736 HCAPLUS
DOCUMENT NUMBER: 115:113736
TITLE: Condensation reaction of N-sulfinylperfluoroalkanesulfonamides
AUTHOR(S): Zhu, Shizheng; Chen, Qingyun
CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, 200032, Peop. Rep. China
SOURCE: Journal of the Chemical Society, Chemical Communications (1991), (10), 732-3
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:113736
AB N-Sulfinylperfluoroalkanesulfonamides, RfSO2NSO, which are prepared by refluxing perfluoroalkanesulfonamides with SOCl2, react easily with aldehydes, ketones, sulfoxides, and POCl3 to yield a series of new compds. RfSO2N:Y [Y = PhCH, cyclohexylidene, R1R2S [R1 = R2 = Me; R1R2 = (CH2)4, PCl3] with elimination of SO2.
CC 21-2 (General Organic Chemistry)
IT **135705-80-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation reaction of, with carbonyl compds., sulfoxides, or phosphorus oxychloride)
IT **67-68-5P**, Dimethyl sulfoxide, preparation **100-52-7P**, Benzaldehyde, reactions 108-93-0P, Cyclohexanol, reactions 1600-44-8P 10025-87-3P, Phosphorus oxychloride
RL: **RCT (Reactant)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**
(condensation reaction of, with N-sulfinylperfluoroalkenesulfonamide)
IT **135705-80-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation reaction of, with carbonyl compds., sulfoxides, or phosphorus oxychloride)
RN 135705-80-5 HCAPLUS
CN Ethanesulfonamide, 1,1,2,2-tetrafluoro-N-sulfinyl-2-(1,1,2,2-tetrafluoroethoxy)- (9CI) (CA INDEX NAME)



IT **67-68-5P**, Dimethyl sulfoxide, preparation **100-52-7P**, Benzaldehyde, reactions
RL: **RCT (Reactant)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**
(condensation reaction of, with N-sulfinylperfluoroalkenesulfonamide)
RN 67-68-5 HCAPLUS
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)



RN 100-52-7 HCAPLUS
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



L27 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:35271 HCAPLUS
DOCUMENT NUMBER: 112:35271
TITLE: Generation and reactions of novel copper carbenoids through a stoichiometric reaction of copper metal with gem-dichlorides in dimethyl sulfoxide
AUTHOR(S): Tezuka, Yasuyuki; Hashimoto, Akio; Ushizaka, Koh; Imai, Kiyokazu
CORPORATE SOURCE: Dep. Mater. Sci. Technol., Nagaoka Univ. Technol., Nagaoka, 940-21, Japan
SOURCE: Journal of Organic Chemistry (1990), 55(1), 329-33
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:35271

AB Copper metal and such gem-dichlorides as α,α-dichloro acid esters X2CRCO2R1 (I; X = Cl, Br; R = H, Me; R1 = alkyl, Ph), Ph2Cl2 (II), PhCHCl2 (III), MeCOCHCl2 (IV), MeCH:CHCHCl2 (V), and CCl4 (VI) were found to undergo a stoichiometric reaction in DMSO under mild conditions to produce copper carbenoid intermediates via α,α-elimination of dichlorides, along with the formation of CuCl2(DMSO)2. Thus, I and II gave substituted olefins via a carbenoid coupling reaction. From V and VI, reaction products were produced via oxygen abstraction from DMSO, together with Me2S; III and IV were found to cause both types of reactions. The carbenoid intermediate formed from I did not cause cyclopropanation reaction with cyclohexene in contrast to the conventional carbalkoxy carbenoid generated by a decomposition reaction of ethyl

diazoacetate. Also, the carbenoid coupling reaction was completely inhibited by the addition of triphenylphosphine, which contrasts to the formation of phosphonium ylide with a carbenoid from Et diazoacetate.

CC 23-17 (Aliphatic Compounds)

IT **100-52-7P**, Benzaldehyde, preparation
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in reaction of benzal chloride with copper metal)

IT **4170-30-3P**, 2-Butenal
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by reaction of dichlorobutene with copper metal)

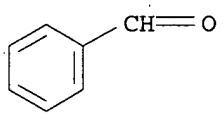
IT 56-23-5, Carbon tetrachloride, reactions **98-87-3**, Benzal chloride **116-54-1 513-88-2 535-15-9**
2051-90-3, Dichlorodiphenyl methane **6482-26-4**, Methyl dibromoacetate **10565-20-5** 17640-03-8 **49653-47-6**
56800-09-0, 1,1-Dichloro-2-butene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with copper metal)

IT **67-68-5**, DMSO, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(solvent, for reaction of copper metal with gem-dichlorides)

IT **100-52-7P**, Benzaldehyde, preparation
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in reaction of benzal chloride with copper metal)

RN 100-52-7 HCAPLUS

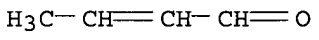
CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **4170-30-3P**, 2-Butenal
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by reaction of dichlorobutene with copper metal)

RN 4170-30-3 HCAPLUS

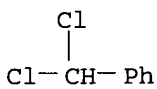
CN 2-Butenal (9CI) (CA INDEX NAME)



IT **98-87-3**, Benzal chloride **116-54-1 513-88-2**
535-15-9 6482-26-4, Methyl dibromoacetate
10565-20-5 49653-47-6 56800-09-0,
1,1-Dichloro-2-butene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with copper metal)

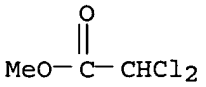
RN 98-87-3 HCAPLUS

CN Benzene, (dichloromethyl)- (9CI) (CA INDEX NAME)

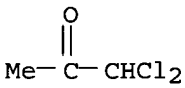


RN 116-54-1 HCAPLUS

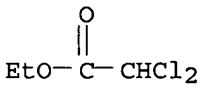
CN Acetic acid, dichloro-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



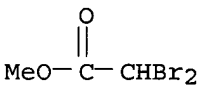
RN 513-88-2 HCAPLUS
CN 2-Propanone, 1,1-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



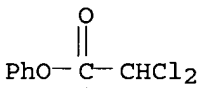
RN 535-15-9 HCAPLUS
CN Acetic acid, dichloro-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



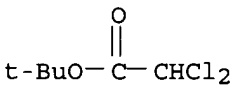
RN 6482-26-4 HCAPLUS
CN Acetic acid, dibromo-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



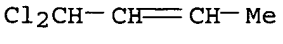
RN 10565-20-5 HCAPLUS
CN Acetic acid, dichloro-, phenyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



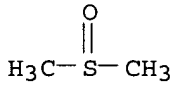
RN 49653-47-6 HCAPLUS
CN Acetic acid, dichloro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



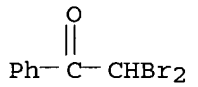
RN 56800-09-0 HCAPLUS
CN 2-Butene, 1,1-dichloro- (9CI) (CA INDEX NAME)



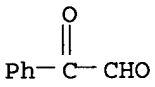
IT **67-68-5**, DMSO, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(solvent, for reaction of copper metal with gem-dichlorides)
RN 67-68-5 HCAPLUS
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)



L27 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:43362 HCAPLUS
DOCUMENT NUMBER: 86:43362
TITLE: Study of the reaction of dimethyl sulfoxide with bromo- and dibromomethyl aryl ketones
AUTHOR(S): Saldabols, N.; Cimanis, A.; Hillers, S.
CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
SOURCE: Tezisy Dokl. Nauchn. Sess. Khim. Tekhnol. Org. Soedin. Sery Sernistykh Neftei, 13th (1974), 188. Editor(s): Gal'pern, G. D. "Zinatne": Riga, USSR.
CODEN: 33SUAA
DOCUMENT TYPE: Conference
LANGUAGE: Russian
AB Oxidation of BrCH2COR (R = aryl) with Me2SO gave RCOCHO and RCOCO2Me. Reaction of Br2CHCOR with Me2SO gave an intermediate arylmethoxysulfonium salt, which was easily decomposed to give Me2S and RCOCOBr; MeSO3H and Me3S+ Br- were also isolated from the reaction mixture
CC 25-17 (Noncondensed Aromatic Compounds)
IT 70-11-1 **13665-04-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of, with dimethyl sulfoxide)
IT **1074-12-0DP**, derivs. 15206-55-0DP, derivs.
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **67-68-5**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with bromo-and dibromomethyl aryl ketones)
IT **13665-04-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of, with dimethyl sulfoxide)
RN 13665-04-8 HCAPLUS
CN Ethanone, 2,2-dibromo-1-phenyl- (9CI) (CA INDEX NAME)



IT **1074-12-0DP**, derivs.
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 1074-12-0 HCAPLUS
CN Benzeneacetaldehyde, α-oxo- (9CI) (CA INDEX NAME)



IT **67-68-5**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(with bromo-and dibromomethyl aryl ketones)
RN 67-68-5 HCAPLUS
CN Methane, sulfinylbis- (9CI) (CA INDEX NAME)